```
=> d his ful

     (FILE 'HOME' ENTERED AT 14:09:07 ON 25 JUL 2005)

     FILE 'CAPLUS' ENTERED AT 14:09:13 ON 25 JUL 2005
                E US2004-816128/APPS
L1            67 SEA ABB=ON  PLU=ON  BRANDVOLD?/AU
L2             0 SEA ABB=ON  PLU=ON  LEWIS?/AU AND  L1
L3          1218 SEA ABB=ON  PLU=ON  KING L?/AU
L4          1693 SEA ABB=ON  PLU=ON  LEWIS G?/AU
L5             0 SEA ABB=ON  PLU=ON  L3 AND L4
L6             0 SEA ABB=ON  PLU=ON  L1 AND L4
L7           350 SEA ABB=ON  PLU=ON  BREWER L?/AU
L8             1 SEA ABB=ON  PLU=ON  L7 AND (L4 OR L3 OR L1)
                D SCA TI
                E HYDROPEROXIDES/CT
                E E3+ALL
L9          1430 SEA ABB=ON  PLU=ON  HYDROPEROXIDES+PFT,NT/CT(L)PREP+ALL/RL

     FILE 'REGISTRY' ENTERED AT 14:12:04 ON 25 JUL 2005
L10         6069 SEA ABB=ON  PLU=ON  "HYDROPEROXIDE"
L11              STR
L12           50 SEA SSS SAM L11
L13        11585 SEA SSS FUL L11

     FILE 'CAPLUS' ENTERED AT 14:13:19 ON 25 JUL 2005
L14         5326 SEA ABB=ON  PLU=ON  L13(L)PREP+ALL/RL
L15         5810 SEA ABB=ON  PLU=ON  L9 OR L14

     FILE 'REGISTRY' ENTERED AT 14:14:14 ON 25 JUL 2005

     FILE 'CAPLUS' ENTERED AT 14:14:17 ON 25 JUL 2005

     FILE 'REGISTRY' ENTERED AT 14:16:07 ON 25 JUL 2005
L*** DEL         TRA L15 1- RN :    50608 TERMS

     FILE 'REGISTRY' ENTERED AT 14:16:07 ON 25 JUL 2005

     FILE 'CAPLUS' ENTERED AT 14:16:28 ON 25 JUL 2005
L16         1225 SEA ABB=ON  PLU=ON  L15 AND PY>1998
L17         1716 SEA ABB=ON  PLU=ON  L15 AND PY>1995
L18         4094 SEA ABB=ON  PLU=ON  L15 NOT L17

     FILE 'REGISTRY' ENTERED AT 14:17:03 ON 25 JUL 2005

     FILE 'CAPLUS' ENTERED AT 14:17:06 ON 25 JUL 2005
L19              TRA L17 1- RN :    23938 TERMS

     FILE 'REGISTRY' ENTERED AT 14:17:27 ON 25 JUL 2005
L20        23938 SEA ABB=ON  PLU=ON  L19

     FILE 'CAPLUS' ENTERED AT 14:23:58 ON 25 JUL 2005
L21              TRA L18 1- RN :    33989 TERMS

     FILE 'REGISTRY' ENTERED AT 14:24:49 ON 25 JUL 2005
L22        33987 SEA ABB=ON  PLU=ON  L21
L23        54744 SEA ABB=ON  PLU=ON  L20 OR L22
L24          986 SEA ABB=ON  PLU=ON  L23 AND (MN OR CO OR CR OR V OR MO OR FE
```

```
                OR CU OR NI)/ELS
                E OXYGEN/CN
L25           1 SEA ABB=ON  PLU=ON  OXYGEN/CN
                SEL RN
L26         400 SEA ABB=ON  PLU=ON  L25 OR 7782-44-7/CRN

     FILE 'CAPLUS' ENTERED AT 14:28:03 ON 25 JUL 2005
L27      180563 SEA ABB=ON  PLU=ON  L24(L)(CAT/RL OR ?CATAL?)
L28       53387 SEA ABB=ON  PLU=ON  L26(L)RACT+ALL/RL
L29         523 SEA ABB=ON  PLU=ON  L15 AND L27
L30          47 SEA ABB=ON  PLU=ON  L29 AND L28

     FILE 'REGISTRY' ENTERED AT 14:29:08 ON 25 JUL 2005
L*** DEL         STR

     FILE 'CASREACT' ENTERED AT 14:29:48 ON 25 JUL 2005
L31              STR
L32            2 SEA SSS SAM L31 (    10 REACTIONS)
L33           30 SEA SSS FUL L31 (   248 REACTIONS)

     FILE 'STNGUIDE' ENTERED AT 14:34:01 ON 25 JUL 2005


     FILE HOME

     FILE CAPLUS

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     FILE COVERS 1907 - 25 Jul 2005  VOL 143 ISS 5
     FILE LAST UPDATED: 24 Jul 2005  (20050724/ED)

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

       This file contains CAS Registry Numbers for easy and accurate
       substance identification.

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   24 JUL 2005  HIGHEST RN 856767-39-0
     DICTIONARY FILE UPDATES:  24 JUL 2005  HIGHEST RN 856767-39-0

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.
```

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*************************************************************
*                                                           *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                           *
*************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

FILE CASREACT
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FILE CONTENT:1840 - 24 Jul 2005 VOL 143 ISS 4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*********************************************************
*                                                       *
*     CASREACT now has more than 9.2 million reactions  *
*                                                       *
*********************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jul 22, 2005 (20050722/UP).

=> dup rem l33 l30
FILE 'CASREACT' ENTERED AT 14:34:15 ON 25 JUL 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CAPLUS' ENTERED AT 14:34:15 ON 25 JUL 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L33
PROCESSING COMPLETED FOR L30
L34          76 DUP REM L33 L30 (1 DUPLICATE REMOVED)
                ANSWERS '1-30' FROM FILE CASREACT
                ANSWERS '31-76' FROM FILE CAPLUS
```

```
=> d que stat l33
L31             STR

RRT          RRT          PRO              G1 8      Mn @9     Co @10    Cr @11

C~~H         O~~O         C~~O~~OH
1   2        6   7        3   4   5


V @12     Mo @13    Fe @14    Cu @15    Ni @16


VAR G1=9/10/11/12/13/14/15/16
NODE ATTRIBUTES:
NSPEC   IS RC     AT   1
NSPEC   IS RC     AT   3
NSPEC   IS RC     AT   9
NSPEC   IS RC     AT  10
NSPEC   IS RC     AT  11
NSPEC   IS RC     AT  12
NSPEC   IS RC     AT  13
NSPEC   IS RC     AT  14
NSPEC   IS RC     AT  15
NSPEC   IS RC     AT  16
CONNECT IS E1  RC AT   6
CONNECT IS E1  RC AT   7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE

  ****MAPPINGS****
NOD SYM      ROL    NOD SYM      ROL
  1 C        RRT      3 C        PRO
  3 C        PRO      1 C        RRT
L33          30 SEA FILE=CASREACT SSS FUL L31 (   248 REACTIONS)

100.0% DONE    2043 VERIFIED     248 HIT RXNS                    30 DOCS
SEARCH TIME: 00.00.01



=> d que stat l30
L9          1430 SEA FILE=CAPLUS ABB=ON  PLU=ON  HYDROPEROXIDES+PFT,NT/CT(L)PREP
                 +ALL/RL
L11              STR

C~~O~~OH
1   2   3


NODE ATTRIBUTES:
NSPEC   IS RC     AT   1
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

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L13       11585 SEA FILE=REGISTRY SSS FUL L11
L14        5326 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13(L)PREP+ALL/RL
L15        5810 SEA FILE=CAPLUS ABB=ON  PLU=ON  L9 OR L14
L17        1716 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 AND PY>1995
L18        4094 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 NOT L17
L19             TRANSFER  PLU=ON  L17 1- RN :   23938 TERMS
L20       23938 SEA FILE=REGISTRY ABB=ON  PLU=ON  L19
L21             TRANSFER  PLU=ON  L18 1- RN :   33989 TERMS
L22       33987 SEA FILE=REGISTRY ABB=ON  PLU=ON  L21
L23       54744 SEA FILE=REGISTRY ABB=ON  PLU=ON  L20 OR L22
L24         986 SEA FILE=REGISTRY ABB=ON  PLU=ON  L23 AND (MN OR CO OR CR OR V
                OR MO OR FE OR CU OR NI)/ELS
L25           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  OXYGEN/CN
L26         400 SEA FILE=REGISTRY ABB=ON  PLU=ON  L25 OR 7782-44-7/CRN
L27      180563 SEA FILE=CAPLUS ABB=ON  PLU=ON  L24(L)(CAT/RL OR ?CATAL?)
L28       53387 SEA FILE=CAPLUS ABB=ON  PLU=ON  L26(L)RACT+ALL/RL
L29         523 SEA FILE=CAPLUS ABB=ON  PLU=ON  L15 AND L27
L30          47 SEA FILE=CAPLUS ABB=ON  PLU=ON  L29 AND L28
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=> d l34 ibib abs crd 1-30

L34 ANSWER 1 OF 76 CASREACT COPYRIGHT 2005 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 126:343150 CASREACT

TITLE: Preparative Oxidation of Organic Compounds in Microemulsions with Singlet Oxygen Generated Chemically by the Sodium Molybdate/Hydrogen Peroxide System

AUTHOR(S): Aubry, Jean-Marie; Bouttemy, Sabine

CORPORATE SOURCE: Faculte de Pharmacie de Lille, CNRS URA 351, Lille, F-59006, Fr.

SOURCE: Journal of the American Chemical Society (1997), 119(23), 5286-5294
CODEN: JACSAT; ISSN: 0002-7863

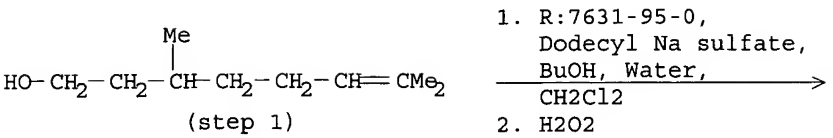
PUBLISHER: American Chemical Society

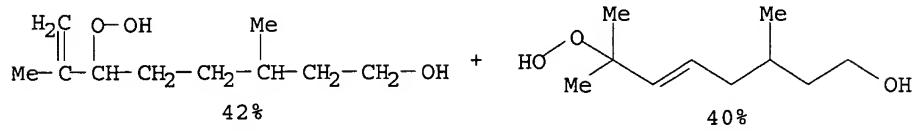
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A reverse (water in oil) microemulsion has been designed to oxidize hydrophobic organic substrates with singlet oxygen (1O2, 1Δg) generated by the disproportionation of hydrogen peroxide catalyzed by molybdate ions. The microemulsion was prepared by mixing methylene chloride, SDS, 1-butanol, and aqueous molybdate. Steady-state and flash photolysis studies have shown that in such media singlet oxygen exhibits a kinetic behavior similar to that under homogeneous conditions ($\tau\Delta \approx 42$ μs). Various typical organic substrates have been oxidized on a preparative scale with this chemical generated singlet oxygen, and the expected oxidation products have been isolated in high yields.

RX(7) OF 10

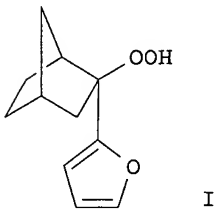




NOTE: SINGLET OXYGEN PREPD. IN SITU BY PEROXIDE INTERACTION WITH MICROEMULSION

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:190557 CASREACT
TITLE: Synthesis of a renewable hydroperoxide from (+)-norcamphor: influence of steric modifications of the bicyclic framework on asymmetric sulfoxidation
AUTHOR(S): Lattanzi, Alessandra; Iannece, Patrizia; Scettri, Arrigo
CORPORATE SOURCE: Dipartimento di Chimica, Universita degli Studi di Salerno, Baronissi (SA), 84081, Italy
SOURCE: Tetrahedron: Asymmetry (2004), 15(11), 1779-1785
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

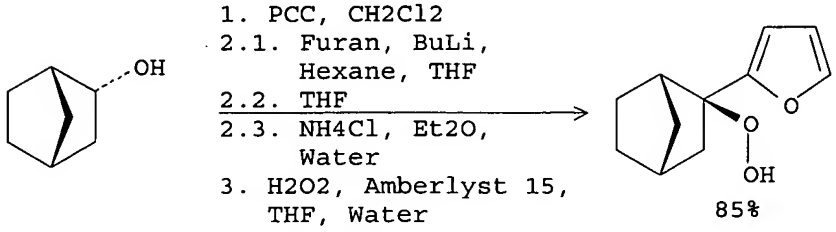


I

AB A renewable tertiary hydroperoxide I has been efficiently synthesized in 83% overall yield starting from com. available (+)-endo-2-norborneol. This oxygen donor, derived from (+)-norcamphor, when employed in Ti(OCHMe2)4-catalyzed oxidns. of sulfides to sulfoxides, proved to be considerably more reactive when compared to a previously reported camphor-derived hydroperoxide. Reduced steric hindrance of the new oxidant lowered the level of asym. induction achieved in the oxidation, but stereoconvergent kinetic resolution has been exploited to improve

enantioselectivity. Excellent recovery (95%) of the tertiary alc., (+)-exo-2-furyl-2-norborneol, at the end of the oxidation provides a highly advantageous chiral resource saving protocol.

RX(18) OF 20 - 3 STEPS



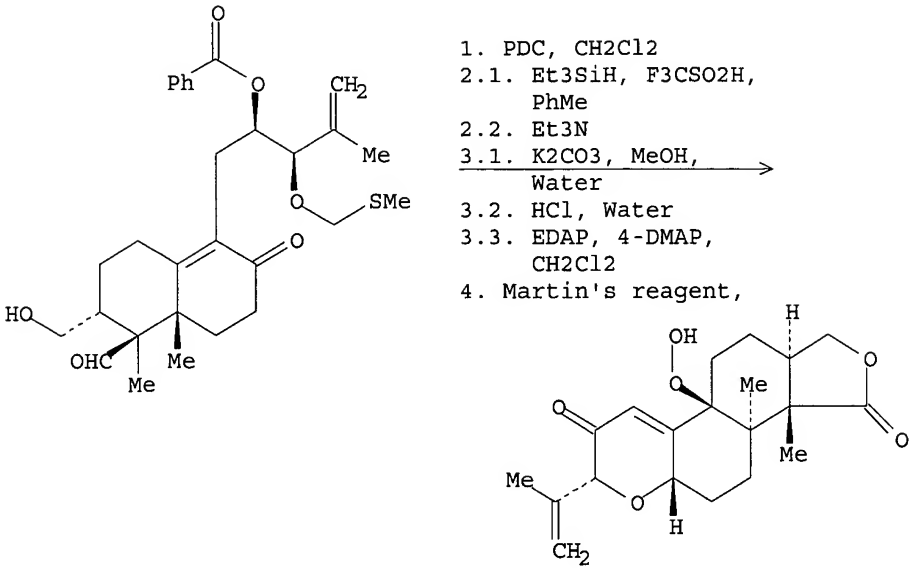
85%

NOTE: 1) mol. sieves used, 3) stereoselective

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

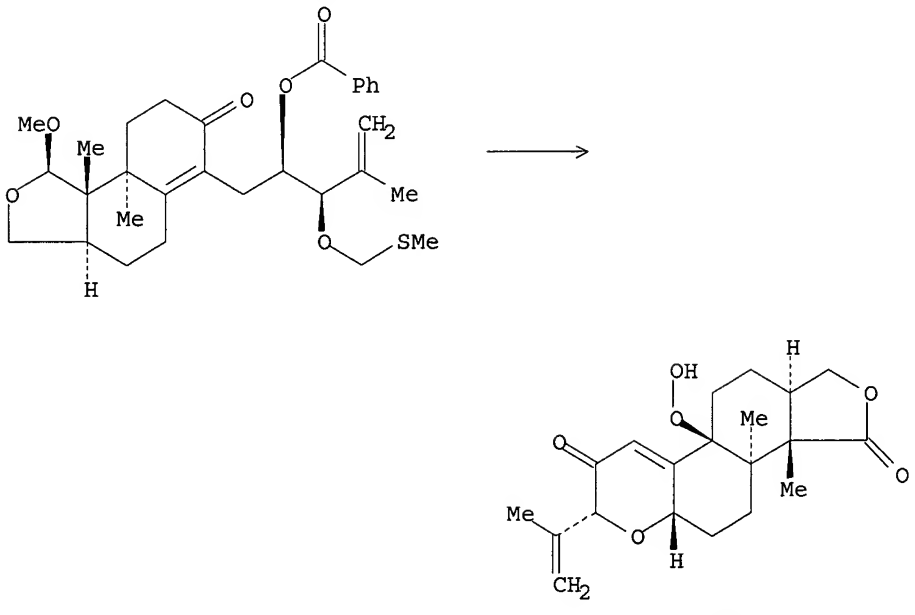
L34 ANSWER 3 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:164895 CASREACT
TITLE: Tremorgenic Indole Alkaloids. The Total Synthesis of (-)-Penitrem D
AUTHOR(S): Smith, Amos B.; Kanoh, Naoki; Ishiyama, Haruaki; Minakawa, Noriaki; Rainier, Jon D.; Hartz, Richard A.; Cho, Young Shin; Cui, Haifeng; Moser, William H.
CORPORATE SOURCE: Department of Chemistry, Monell Chemical Senses Center, and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of the American Chemical Society (2003), 125(27), 8228-8237
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A convergent, stereocontrolled total synthesis of the architecturally complex tremorgenic indole alkaloid (-)-penitrem D was achieved. Highlights of the synthesis include an efficient, asym. synthesis of the western hemisphere; the stereocontrolled assembly of the I-ring; discovery of a novel autoxidn. to introduce the C(22) tertiary hydroxyl group, required for tremorgenic activity; union of fully elaborated eastern and western hemispheres, exploiting an indole synthetic protocol developed expressly for this purpose; and a late-stage, stereoselective construction of the A and F rings exploiting a Sc(OTf)3-promoted reaction cascade. The longest linear sequence leading to (-)-penitrem D was 43 steps.

RX(450) OF 754 - 5 STEPS



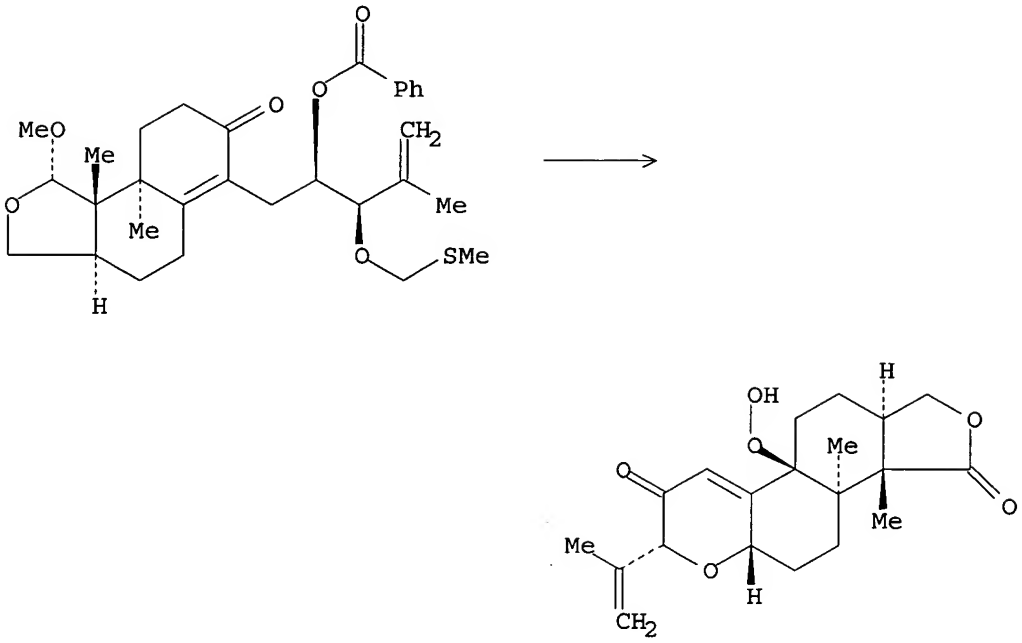
NOTE: 2) stereoselective

RX(452) OF 754 - 6 STEPS



NOTE: 3) stereoselective

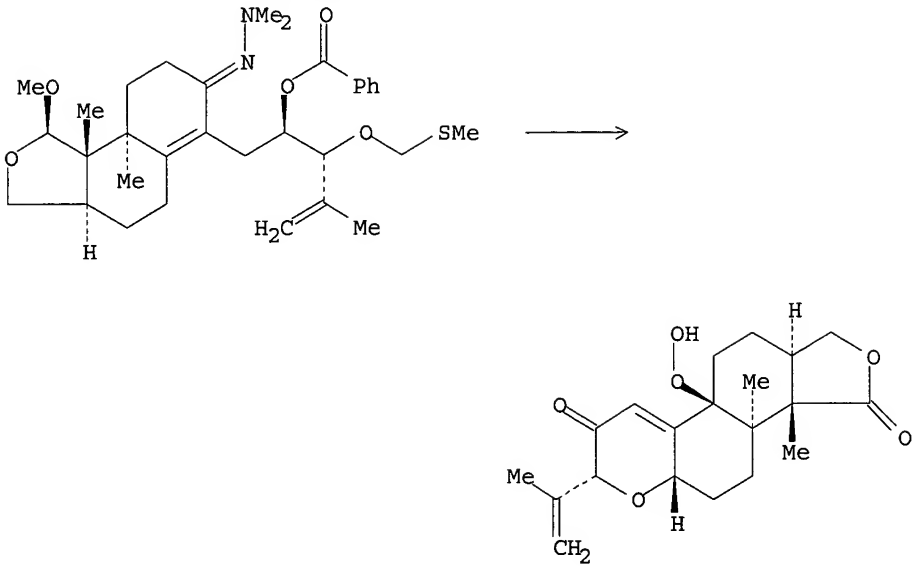
RX(454) OF 754 - 6 STEPS



72%

NOTE: 3) stereoselective

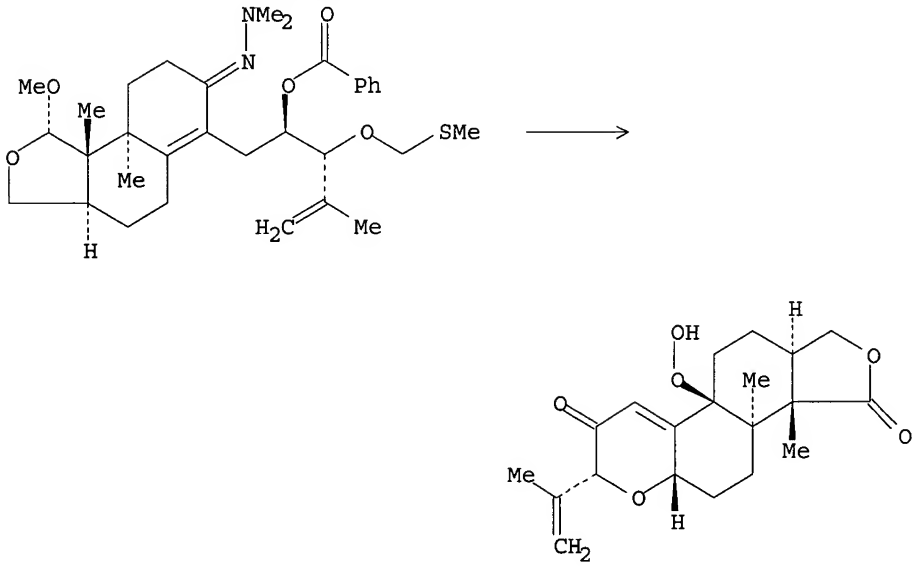
RX(456) OF 754 - 7 STEPS



72%

NOTE: 1) buffered soln. used first stage, 4) stereoselective

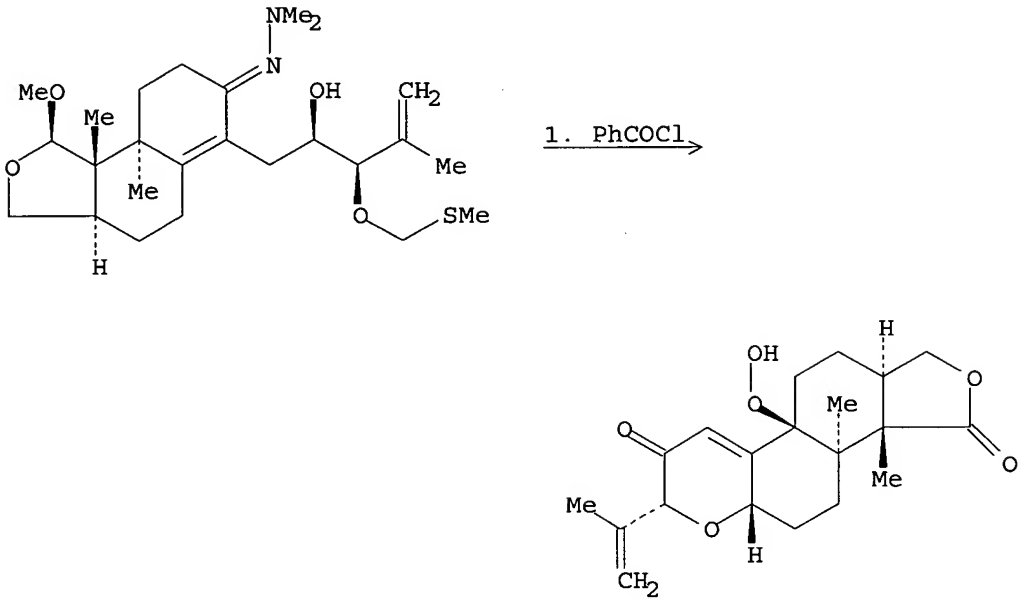
RX(458) OF 754 - 7 STEPS



72%

NOTE: 1) buffered soln. used first stage, 4) stereoselective

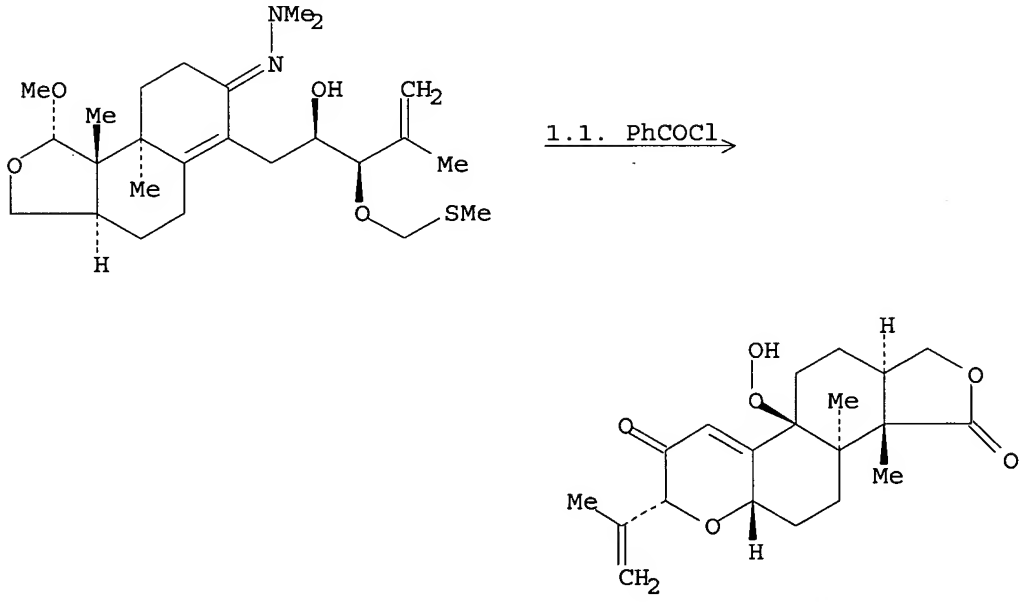
RX(580) OF 754 - 8 STEPS



72%

NOTE: 2) buffered soln. used first stage, 5) stereoselective

RX(581) OF 754 - 8 STEPS



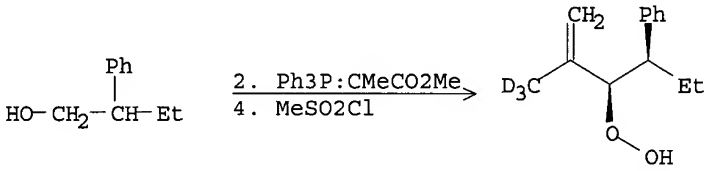
72%

NOTE: 2) buffered soln. used first stage, 5) stereoselective

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 4 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:323158 CASREACT
TITLE: Remarkable Change of the Diastereoselection in the Dye-Sensitized Ene Hydroperoxidation of Chiral Alkenes by Zeolite Confinement
AUTHOR(S): Stratakis, Manolis; Kalaitzakis, Dimitris; Stavroulakis, Dimitris; Kosmas, Giannis; Tsangarakis, Constantinos
CORPORATE SOURCE: Department of Chemistry, University of Crete, Iraklion, 71409, Greece
SOURCE: Organic Letters (2003), 5(19), 3471-3474
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ene reaction of singlet oxygen with chiral trisubstituted alkenes bearing an alkyl and a Ph group at the stereogenic center is erythro diastereoselective in solution and threo diastereoselective if carried out within zeolite Na-Y. The change of the diastereoselectivity trend by zeolite confinement is attributed to a synergism of steric effects and cation-π interactions.

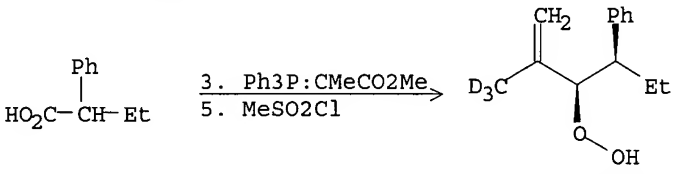
RX(72) OF 76 - 6 STEPS



stereoisomers

NOTE: 2) stereoselective, 6) regioselective, stereoselective, photochem., Na-Y zeolite used

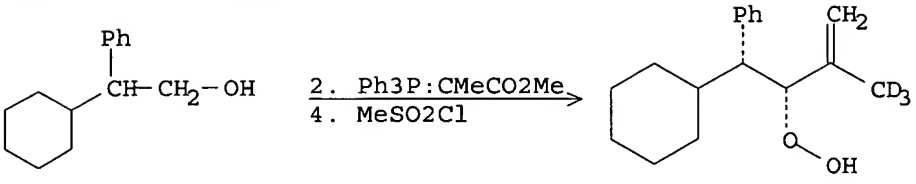
RX(73) OF 76 - 7 STEPS



stereoisomers

NOTE: 3) stereoselective, 7) regioselective, stereoselective, photochem., Na-Y zeolite used

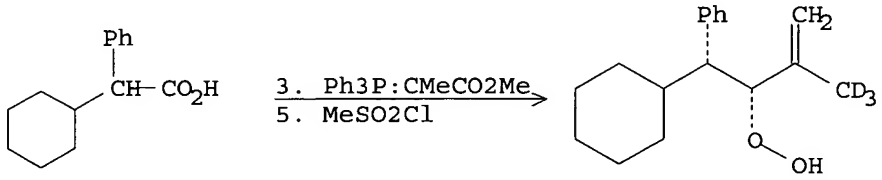
RX(75) OF 76 - 6 STEPS



stereoisomers

NOTE: 2) stereoselective, 6) regioselective, stereoselective, photochem., Na-Y zeolite used

RX(76) OF 76 - 7 STEPS



stereoisomers

NOTE: 3) stereoselective, 7) regioselective, stereoselective, photochem., Na-Y zeolite used

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:133800 CASREACT

TITLE: Asymmetric synthesis with 6-tert-butyl-5-methoxy-6-methyl-3,6-dihydro-2H-1,4-oxazin-2-one as a new chiral glycine equivalent: preparation of enantiomerically pure α-tertiary and α-quaternary α-amino acids

AUTHOR(S): Koch, Claus-Jurgen; Simonyiova, Sona; Pabel, Jorg; Kartner, Annerose; Polborn, Kurt; Wanner, Klaus Theodor

CORPORATE SOURCE: Department Pharmazie - Zentrum fur Pharmaforschung, LMU Munchen, Munchen, 81377, Germany

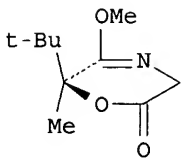
SOURCE: European Journal of Organic Chemistry (2003), (7), 1244-1263
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



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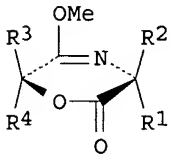
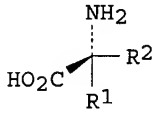
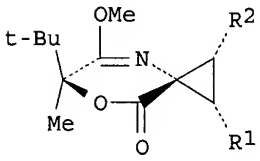


II



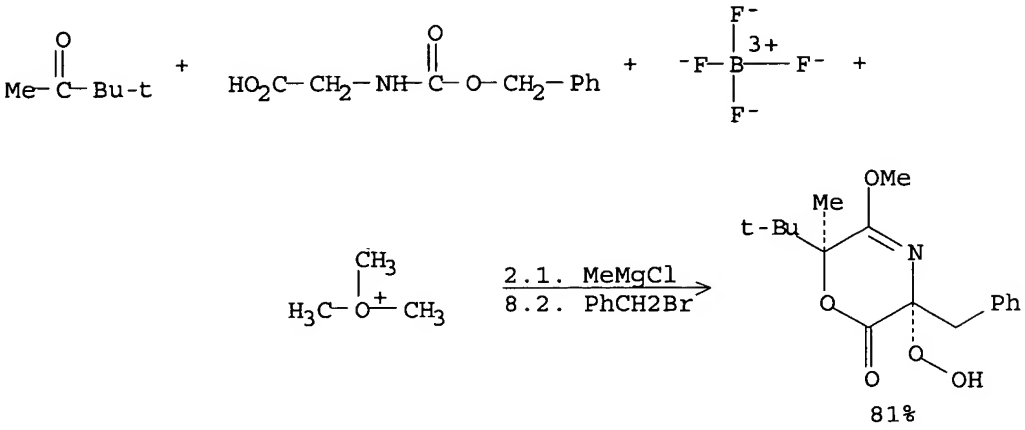
III



IV

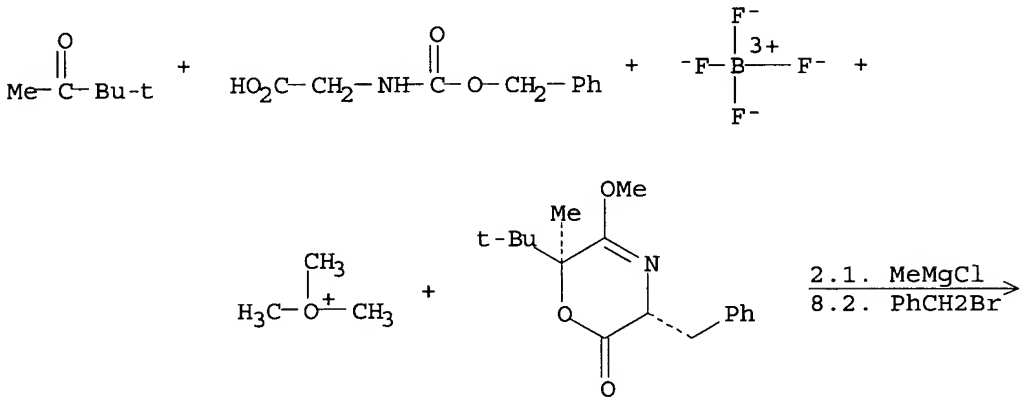
AB The chiral oxazinone I has been developed as a new chiral glycine equivalent for the asym. synthesis of mono- and disubstituted α-amino acids. It is derived from the α-hydroxy-carboxylic acid, which serves as a chiral auxiliary, and is easily accessible in enantiomerically pure form by optical resolution of the racemic compound (RS)-2-hydroxy-2,3,3-trimethylbutanoic acid. For alkylation reactions, I was deprotonated with sBuLi or phosphazenic base. Subsequent treatment with alkyl halides yielded the monosubstituted compds. II (R1 = CH2Ph, CH2CH:CH2, Me, n-Bu, iso-Pr, R2 = H, R3 = tert-Bu, R4 = Me; R1 = H, R2 = CH2Ph, CH2CH:CH2, Me, n-Bu, i-Pr; R3 = tert-Bu, R4 = Me) and (ent)-II (R1 = H, R2 = 13CH3, R3 = Me, R4 = t-Bu; R1 = 13CH3, R2 = H, R3 = Me, R4 = t-Bu), while a second alkylation step, via the corresponding enolates, provided the disubstituted compds. II (R1 = CH2CH:CH2, Me, n-Bu, iso-Pr, R2 = CH2Ph, R3 = tert-Bu, R4 = Me; R1 = CH2Ph, R2 = CH2CH:CH2, Me, n-Bu, iso-Pr, R3 = tert-Bu, R4 = Me). Both alkylation steps proceeded with good yields and excellent diastereoselectivities (up to 99% de) and even less reactive electrophiles such as iso-Pr iodide could be used. The results obtained in this reaction supported the assumption that the enolate of I, as well as those of the monosubstituted derivs. of I, have less tendency to form the aggregates that hamper alkylation reactions with other systems with higher oxygen content. From the major diastereomers of both the mono- and the disubstituted derivs. of I the corresponding α-amino acids III (R1 = CH2Ph, CH2CH:CH2, Me, R2 = H; R1 = CH2CH:CH2, Me, n-Bu, iso-Pr, R2 = CH2Ph) were obtained in high enantiomeric purity by hydrolytic cleavage of the oxazinone ring, accomplished either in two steps with aqueous TFA and aqueous NaOH or in one with either aqueous NaOH or 3 N HBr. Alkylation of the enolate ions of (S)-I or (R)-I with epichlorohydrins as bifunctional electrophiles provided the hydroxymethylenecyclopropyl derivs. IV (R1 = CH2OH, R2 = H; R1 = H, R2 = CH2OH). Hydrolysis of IV (R1 = CH2OH, R2 = H; R1 = H, R2 = CH2OH) afforded the free (1R,2S)- and (1R,2R)-1-amino-2-(hydroxymethyl)cyclopropanecarboxylic acids. Reductive amination with aniline after oxidation of IV (R1 = CH2OH, R2 = H; R1 = H, R2 = CH2OH) to the corresponding aldehydes provided the compds. IV (R1 = CH2NHPh, R2 = H; R1 = H, R2 = CH2NHPh), whereas Mitsunobu treatment of IV (R1 = CH2OH, R2 = H; R1 = H, R2 = CH2OH) with 1-phenyl-3-(trifluoroacetyl)urea afforded the urea derivs. Hydrolysis of these compds. yielded the (1R,2R)- and (1S,2S)-1-amino-2-(phenylaminomethyl)cyclopropanecarboxylic acids, and (1R,2R)-1-amino-2-(aminomethyl)cyclopropanecarboxylic acid.

RX(665) OF 750 - 9 STEPS

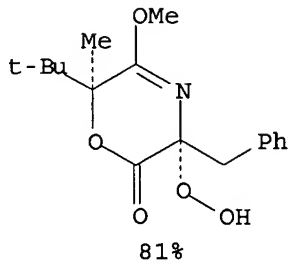


NOTE: 3) stereoselective, 7) buffered soln. used stage 2, 8) stereoselective, yields depend on reaction conditions, 9) buffered soln. used stage 3

RX(693) OF 750 - 10 STEPS



RX(693) OF 750 - 10 STEPS

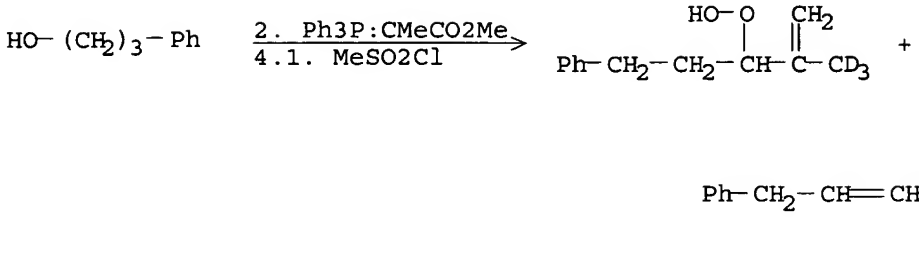


NOTE: 3) stereoselective, 7) buffered soln. used stage 2, 8) stereoselective, yields depend on reaction conditions, 10) buffered soln. used stage 3

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

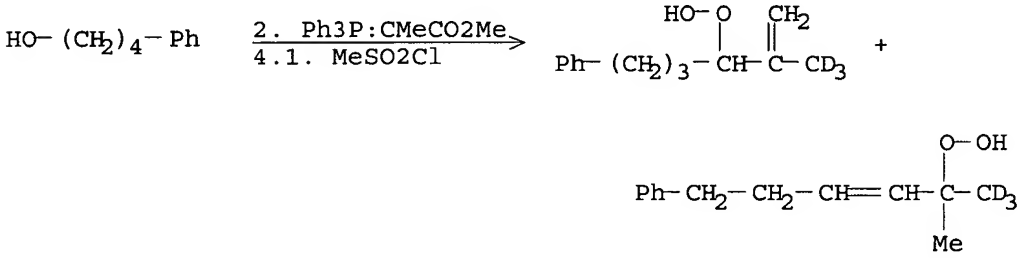
L34 ANSWER 6 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:55585 CASREACT
TITLE: Thionin-Sensitized Intrazeolite Photooxygenation of Trisubstituted Alkenes: Substituent Effects on the Regioselectivity As Probed through Isotopic Labeling
AUTHOR(S): Stratakis, Manolis; Nencka, Radim; Rabalakos, Constantinos; Adam, Waldemar; Krebs, Oliver
CORPORATE SOURCE: Department of Chemistry, University of Crete, Iraklion, 71409, Greece
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8758-8763
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The regioselectivity for the intrazeolite photooxygenation of several trisubstituted alkenes with geminal di-Me groups was examined The length of the alkyl chain at the lone position was varied, and as end groups, the Ph or the cyclohexyl functionalities were chosen. The general trend for all alkenes is a significant increase of the reactivity at the twin position compared to the photooxygenation in solution For the cyclohexyl-substituted alkenes, it was found that the regioselectivity is nearly independent of the alkyl chain length. However, for the phenyl-substituted alkenes, the ene reactivity of the allylic methylene hydrogen atoms at the lone position and the twix/twin regioselectivity depend significantly on the distance of the Ph group from the double bond. These trends are discussed in terms of cation-π interactions and conformational effects. Intramol. and intermol. isotope effects in the intrazeolite photooxygenation of deuterium-labeled alkenes suggest that a perepoxide-type intermediate is formed in the rate-determining step. Type I photooxygenation that involves reaction of the radical cations of the alkenes with superoxide ion are unlikely.

RX(126) OF 141 - 6 STEPS



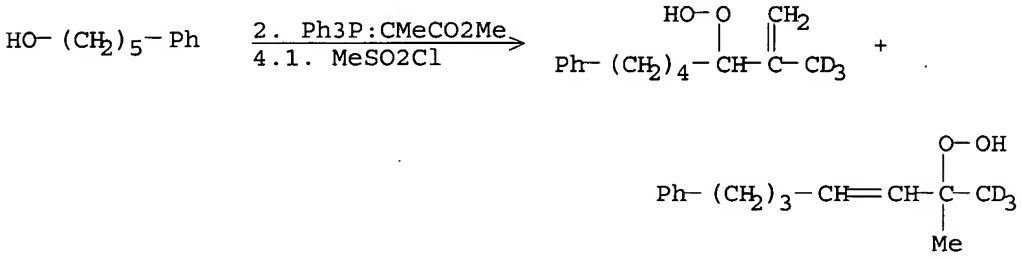
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(129) OF 141 - 6 STEPS



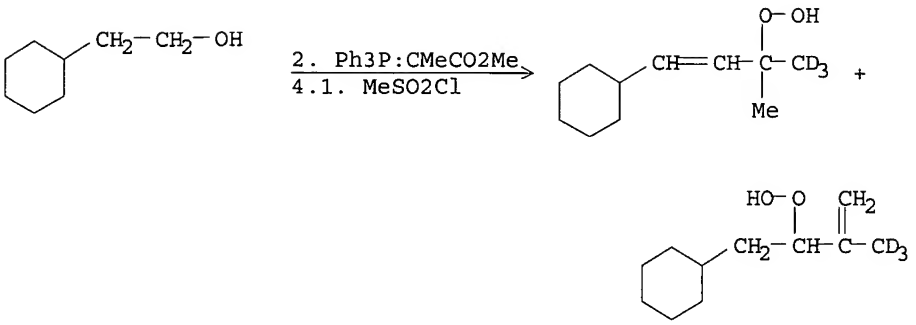
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(132) OF 141 - 6 STEPS



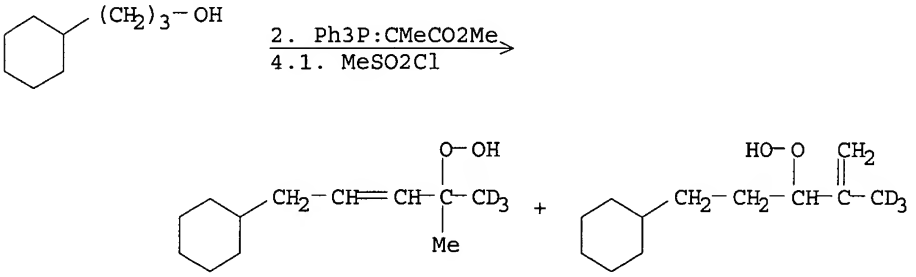
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(135) OF 141 - 6 STEPS



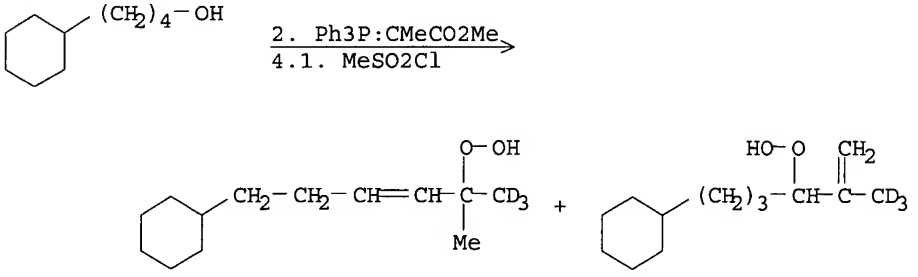
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

RX(138) OF 141 - 6 STEPS



NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

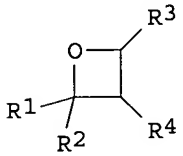
RX(141) OF 141 - 6 STEPS



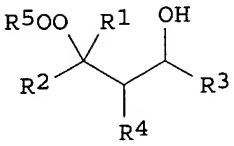
NOTE: 2) stereoselective, 6) thionin-supported zeolite Na-Y used in first stage, photochem. in second stage

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

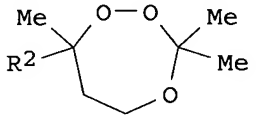
L34 ANSWER 7 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:137276 CASREACT
TITLE: Opening of Substituted Oxetanes with H2O2 and Alkyl Hydroperoxides: Stereoselective Approach to 3-Peroxyalcohols and 1,2,4-Trioxepanes
AUTHOR(S): Dussault, Patrick H.; Trullinger, Tony K.; Noor-e-Ain, Farhana
CORPORATE SOURCE: Department of Chemistry, University of Nebraska Lincoln, Lincoln, NE, 68588-0304, USA
SOURCE: Organic Letters (2002), 4(26), 4591-4593
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



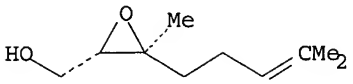
II



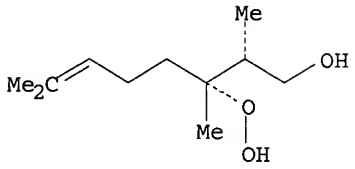
III

AB Lewis acid-catalyzed ring opening of optically active oxetanes I [R1 = R3 = R4 = H, R2 = n-hexyl; R1 = Me, R2 = n-C16H33, Me2C:CHCH2CH2, Me2CH(CH2)3; R3, R4 = H, Me] by hydrogen peroxide proceeded regioselectively and with good to moderate stereoselectivity to furnish enantiomerically enriched 3-hydroperoxyalkanols II (R5 = H). The analogous opening using alkyl hydroperoxides R5O2H (R5 = Me3C, cumyl, tetrahydropyranyl) furnished the corresponding 3-peroxyalkanols II. II (R1 = Me; R2 = n-C16H33, Me2C:CHCH2CH2; R3 = R4 = R5 = H) were easily converted into enantiomerically enriched 1,2,4-trioxepanes III, the building blocks for antimalarials.

RX(65) OF 76 - 3 STEPS



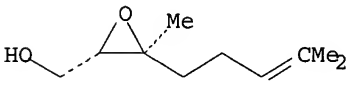
1.1. MeLi, CuI, Et2O
1.2. NH4Cl, Water
2.1. t-BuOK, TsCl, THF
2.2. t-BuOK
3.1. C:54761-04-5, H2O2
3.2. 2,6-Di-t-butylcresol, Water, AcOEt



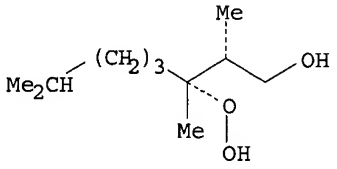
81%

NOTE: 1) stereoselective, 3) regioselective, stereoselective, yield depends on reaction conditions

RX(69) OF 76 - 4 STEPS



1.1. MeLi, CuI, Et2O
1.2. NH4Cl, Water
2. Pd, H2, EtOH
3.1. t-BuOK, TsCl, THF
3.2. t-BuOK
4.1. C:54761-04-5, H2O2, CH2Cl2
4.2. 2,6-Di-t-butylcresol, Water, AcOEt



46%

NOTE: 1) stereoselective, 4) regioselective, stereoselective, product depends on reaction conditions

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

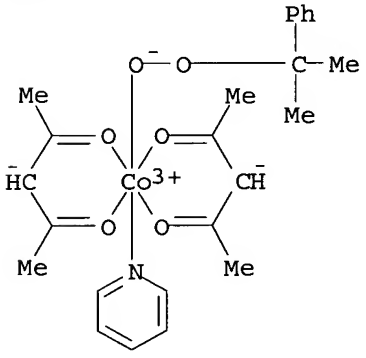
L34 ANSWER 8 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:4635 CASREACT
TITLE: Co(III)-Alkyl Complex- and Co(III)-Alkylperoxo Complex-Catalyzed Triethylsilylperoxidation of Alkenes with Molecular Oxygen and Triethylsilane

AUTHOR(S): Tokuyasu, Takahiro; Kunikawa, Shigeki; Masuyama, Araki; Nojima, Masatomo
CORPORATE SOURCE: Department of Materials Chemistry Frontier Research Center Graduate School of Engineering, Osaka University, Osaka, 565-0871, Japan
SOURCE: Organic Letters (2002), 4(21), 3595-3598
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Both a Co(III)-alkyl complex and a Co(III)-alkylperoxo complex catalyze triethylsilylperoxidn. of alkenes with O2 and Et3SiH. E.g., Co(modp)2 (bis(1-(morpholinocarbamoyl)-4,4-dimethyl-1,3-pentanedionato)cobalt(II)) (shown as I) or Co(acac)2 (II)-catalyzed peroxidn. of H2C:C(CH3)(CH2)2OCOPh proceeded regioselectively affording the triethylsilyl peroxide Et3SiOOC(CH3)2(CH2)2OCOPh in high yield. Although less efficient, cobalt(II) Schiff base complex [Co(SB)] (shown as III) also catalyzed the same reaction. On this basis, together with the non-stereoselectivity in the Co(II)-catalyzed peroxidn. of 3-phenylindene and the formation of the corresponding 1,2-dioxolane from 2-phenyl-1-vinylcyclopropane (a radical clock), the authors propose a reasonable mechanism for the Co(II)-catalyzed novel autoxidn. of alkenes with Et3SiH discovered by Isayama and Mukaiyama.

RX(3) OF 13



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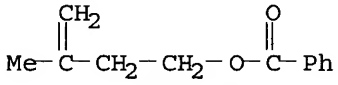
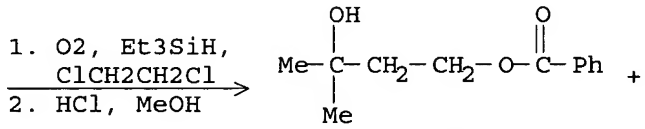
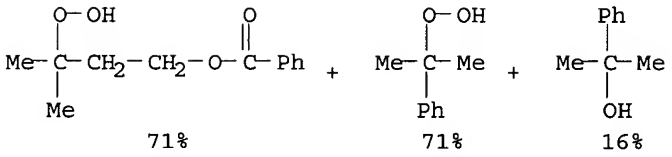


(step 1)



11%

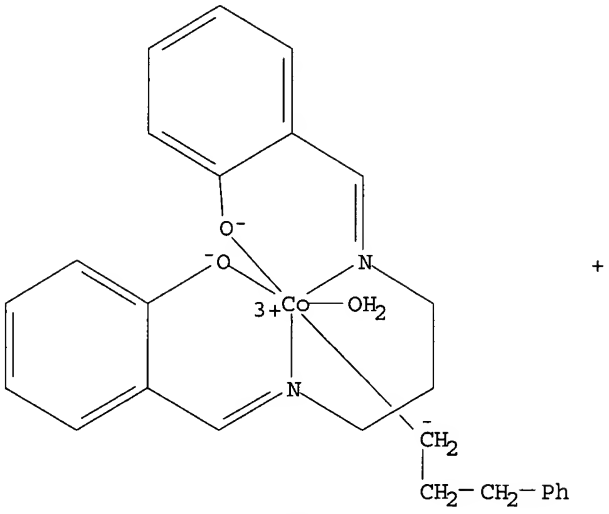
RX(3) OF 13



71% 71% 16%

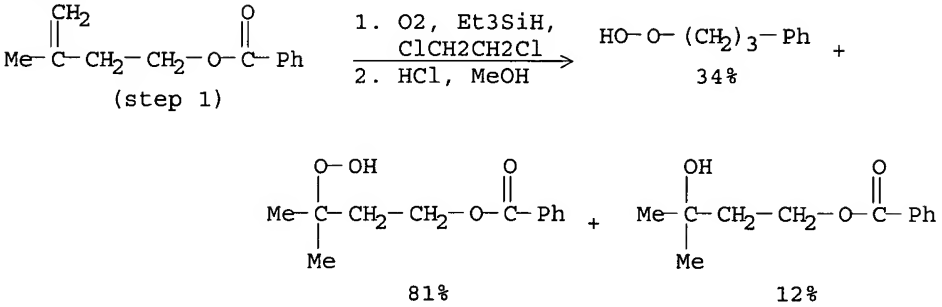
NOTE: room temp., 3 h

RX(6) OF 13



(step 1)

RX(6) OF 13

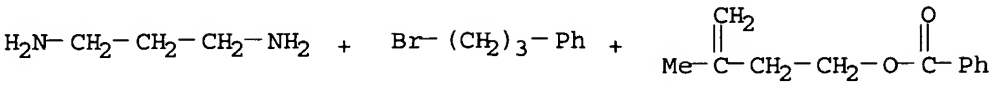


(step 1) 34%

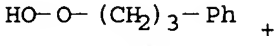
81% 12%

NOTE: regioselective, room temp., 3.5 h

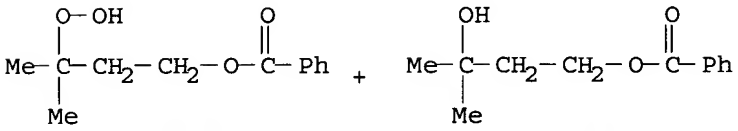
RX(13) OF 13 - 2 STEPS



1.1. 2-HOC6H4CHO, MeOH
1.2. R:7791-13-1
1.3. NaOH, Water
1.4. PdCl2, KCl, NaBH4, Water
2.1. O2, Et3SiH, ClCH2CH2Cl
2.2. HCl, MeOH



34%

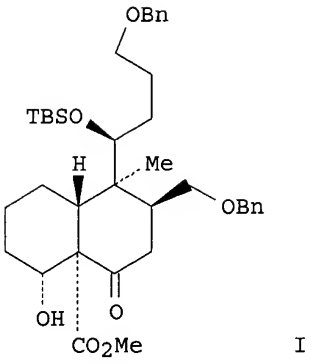


81% 12%

NOTE: 2) regioselective, room temp., 3.5 h

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

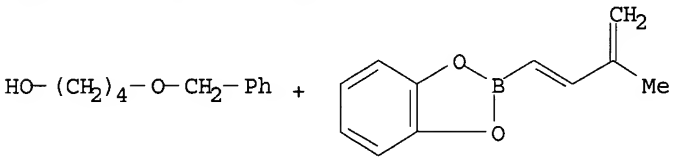
L34 ANSWER 9 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 136:386270 CASREACT
TITLE: A concise synthesis of an advanced clerodin intermediate through a Vaultier tandem reaction
AUTHOR(S): Lallemand, Jean-Yves; Six, Yvan; Ricard, Louis
CORPORATE SOURCE: Laboratoire DCSO. URA 1308 du CNRS, Ecole Polytechnique, Palaiseau, 91128, Fr.
SOURCE: European Journal of Organic Chemistry (2002), (3), 503-513
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



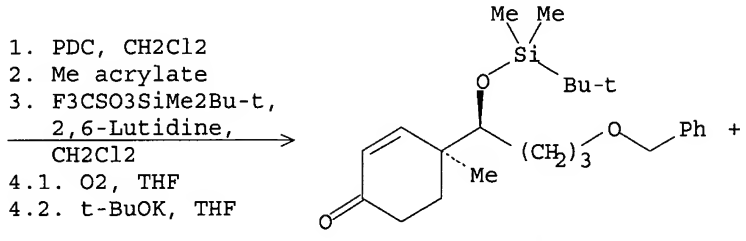
I

AB A highly functionalized precursor (I) of the antifeedant natural product clerodin has been synthesized with good diastereo-control. Key steps include a three-component version of the Vaultier tandem sequence, and an oxidative decarboxylation with a simple exptl. procedure.

RX(58) OF 212 - 4 STEPS

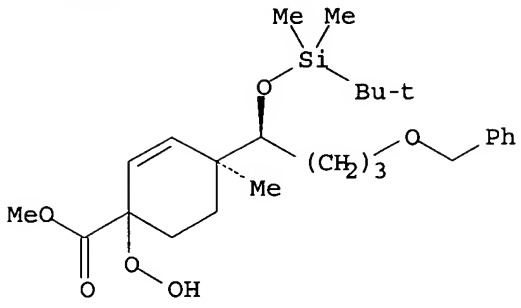


(step 2)



26%

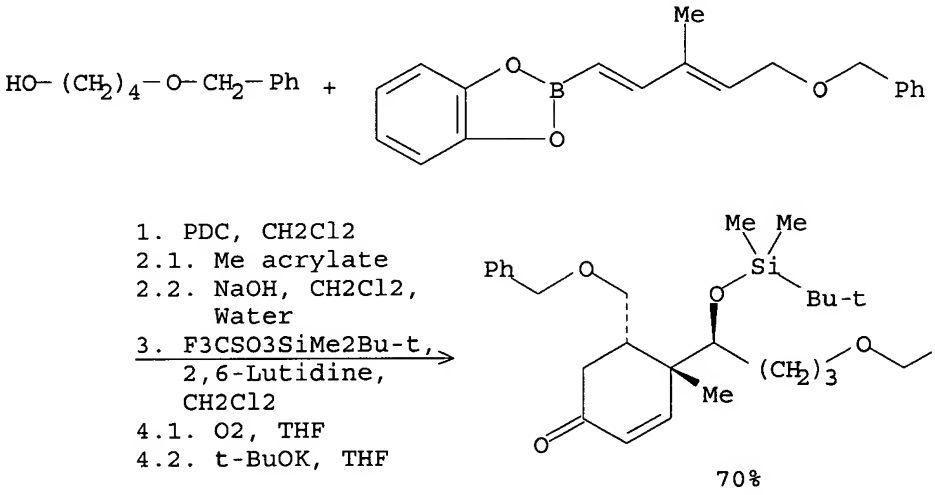
RX(58) OF 212 - 4 STEPS



59%

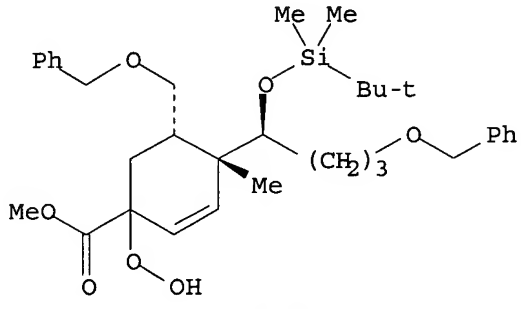
NOTE: 1) Celite used, 2) alternative reaction conditions gave lower yield

RX(66) OF 212 - 4 STEPS



70%

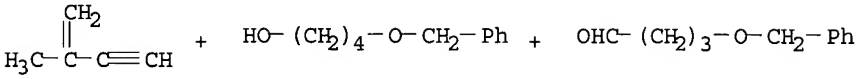
RX(66) OF 212 - 4 STEPS



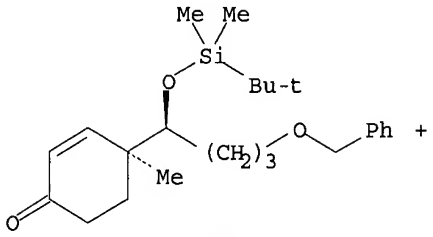
8%

NOTE: 1) Celite used, 2) petroleum ether solvent used

RX(103) OF 212 - 5 STEPS

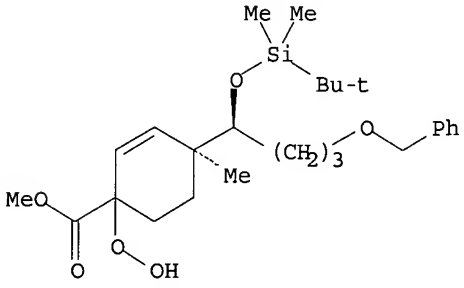


converging
Catecholborane
Me acrylate
F3CSO3SiMe2Bu-t



26%

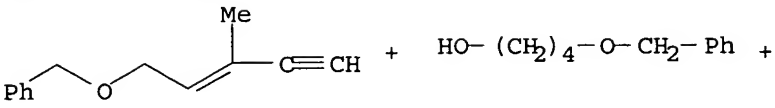
RX(103) OF 212 - 5 STEPS

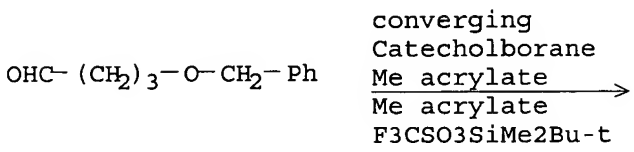


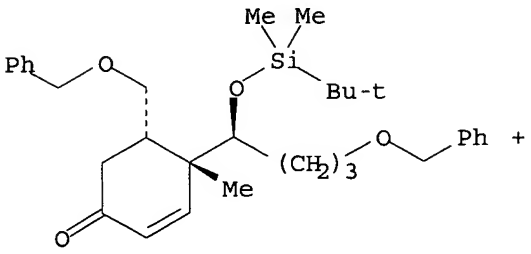
59%

NOTE: alternative reaction conditions gave lower yield, Celite used

RX(139) OF 212 - 5 STEPS

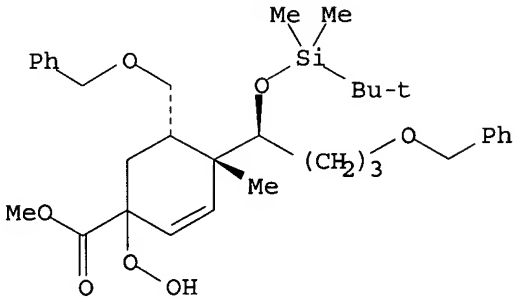






70%

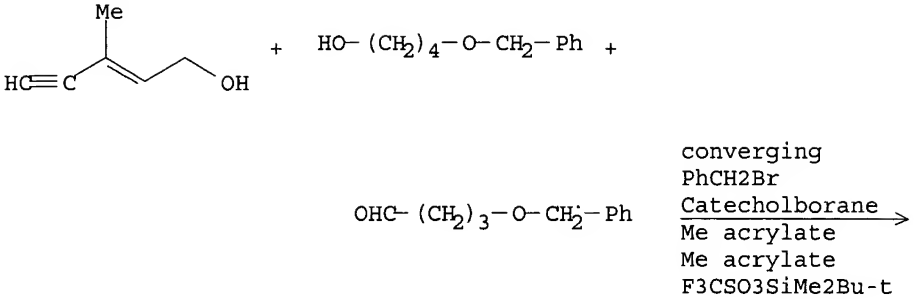
RX(139) OF 212 - 5 STEPS



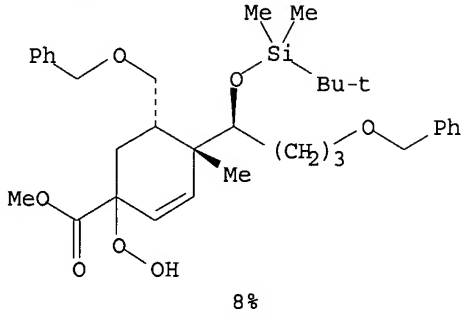
8%

NOTE: petroleum ether solvent used, Celite used

RX(145) OF 212 - 6 STEPS

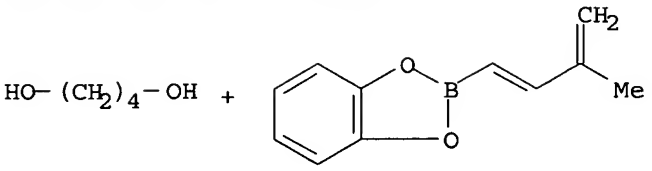


RX(145) OF 212 - 6 STEPS



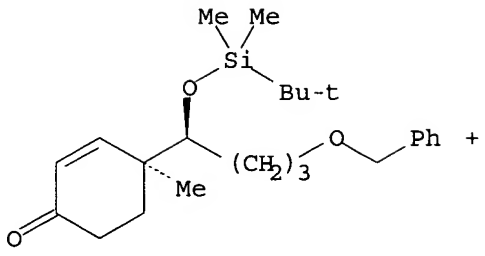
NOTE: petroleum ether solvent used, Celite used

RX(194) OF 212 - 5 STEPS



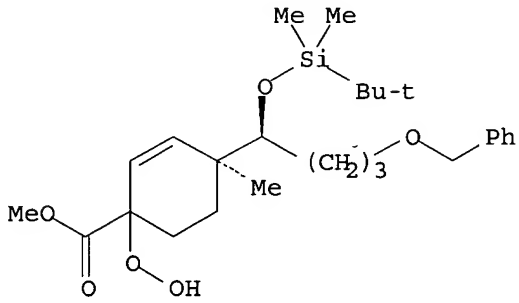
(step 3)

1.1. NaH, THF
1.2. PhCH2Br, Bu4N.I, THF
2. PDC, CH2Cl2
3. Me acrylate
4. F3CSO3SiMe2Bu-t, 2,6-Lutidine, CH2Cl2
5.1. O2, THF
5.2. t-BuOK, THF



26%

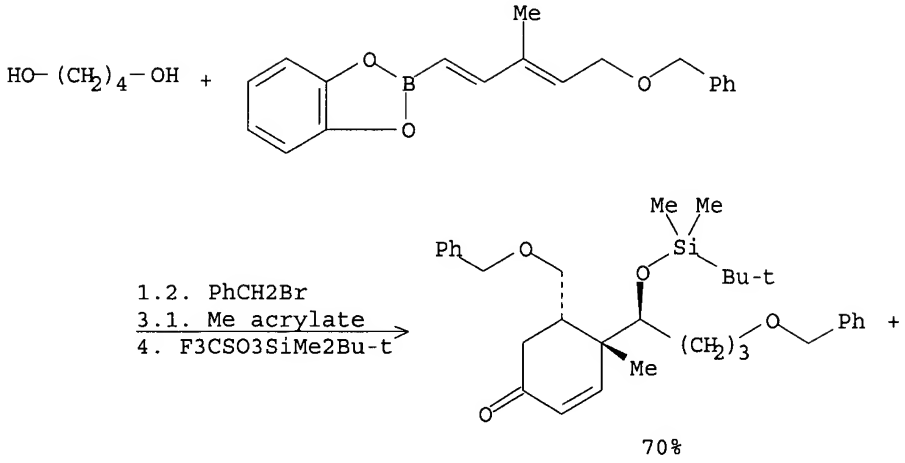
RX(194) OF 212 - 5 STEPS



59%

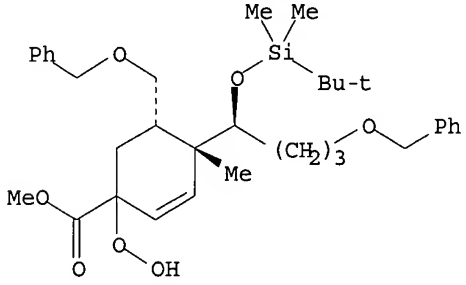
NOTE: 2) Celite used, 3) alternative reaction conditions gave lower yield

RX(195) OF 212 - 5 STEPS



70%

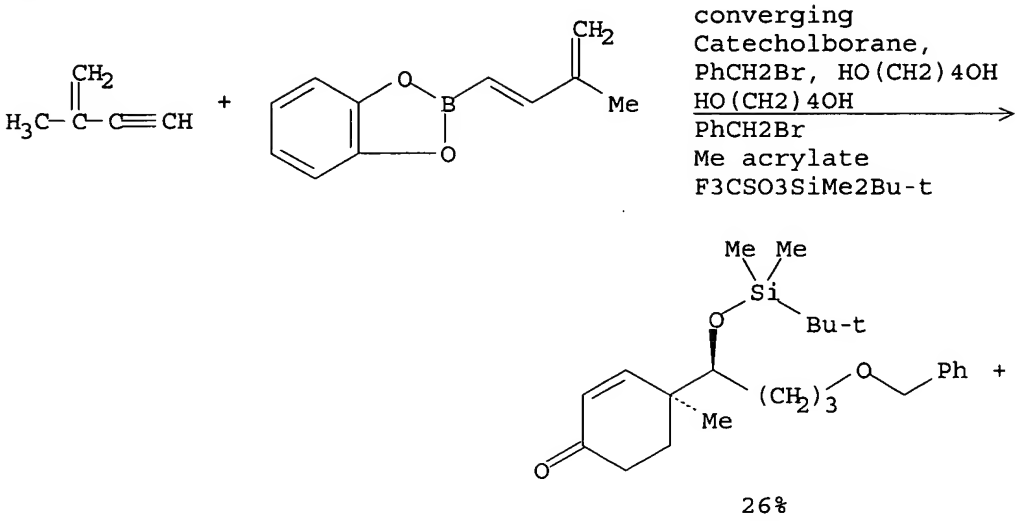
RX(195) OF 212 - 5 STEPS



8%

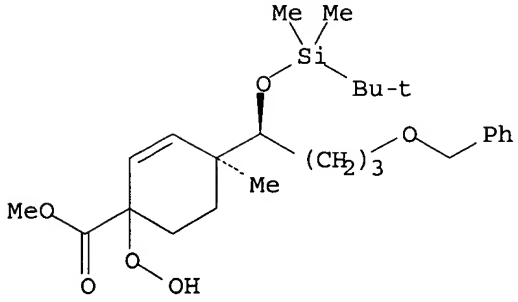
NOTE: 2) Celite used, 3) petroleum ether solvent used

RX(197) OF 212 - 6 STEPS



26%

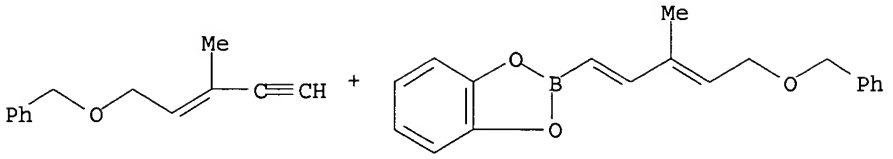
RX(197) OF 212 - 6 STEPS



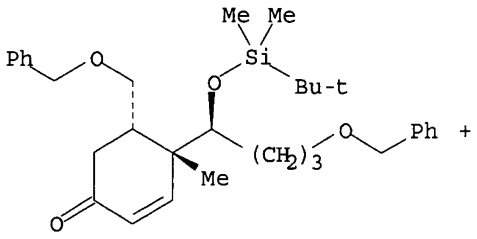
59%

NOTE: Celite used, alternative reaction conditions gave lower yield

RX(198) OF 212 - 6 STEPS

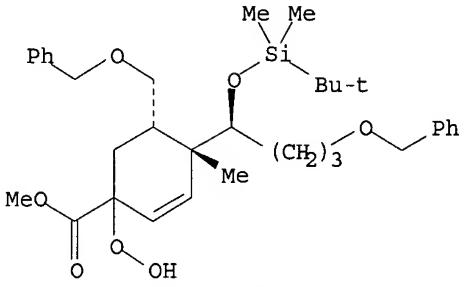


converging
Catecholborane,
PhCH2Br, HO(CH2)4OH
HO(CH2)4OH
PhCH2Br
Me acrylate
Me acrylate
F3CSO3SiMe2Bu-t



70%

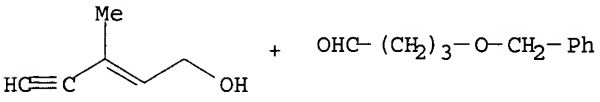
RX(198) OF 212 - 6 STEPS



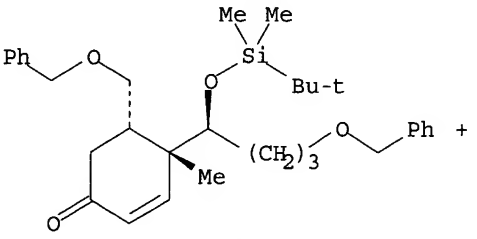
8%

NOTE: Celite used, petroleum ether solvent used

RX(212) OF 212 - 7 STEPS

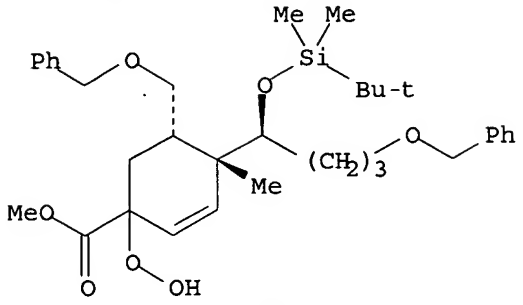


converging
PhCH2Br, HO(CH2)4OH
HO(CH2)4OH
PhCH2Br
Catecholborane
Me acrylate
Me acrylate
F3CSO3SiMe2Bu-t



70%

RX(212) OF 212 - 7 STEPS



8%

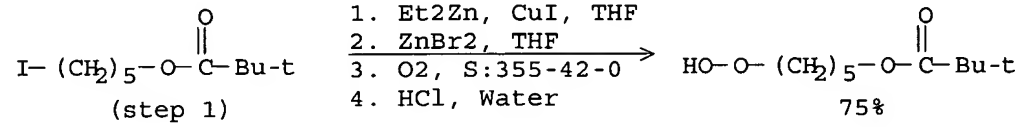
NOTE: petroleum ether solvent used, Celite used

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 10 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 127:161309 CASREACT
TITLE: Chemoselective oxidation of organozinc reagents with oxygen
AUTHOR(S): Klement, Ingo; Lutjens, Henning; Knochel, Paul
CORPORATE SOURCE: Fachbereich Chemie Philipps-Univ., Marburg, D-35032, Germany
SOURCE: Tetrahedron (1997), 53(27), 9135-9144
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

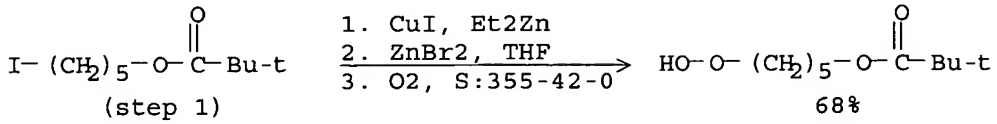
AB Functionalized organozinc compds., prepared by hydrozincation, carbozincation or by boron-zinc exchange, can be directly oxidized in a selective manner to the corresponding functionalized alcs. or hydroperoxides depending on the reaction conditions.

RX(34) OF 42



(step 1) 75%

RX(42) OF 42



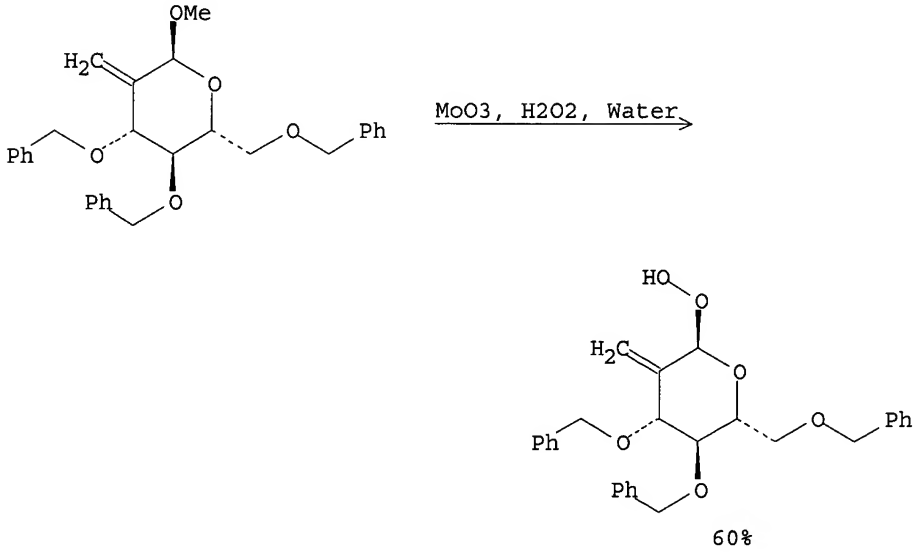
(step 1) 68%

NOTE: safety, pyrophoric reagent, intermediate products could be isolated, chemoselective

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 126:144478 CASREACT
TITLE: New optically pure sugar hydroperoxides. Synthesis and use for enantioselective oxygen transfer
AUTHOR(S): Hamann, Hans-Juergen; Hoeft, Eugen; Mostowicz, Danuta; Mishnev, Anatoly; Urbanczyk-Lipkowska, Zofia; Chmielewski, Marek
CORPORATE SOURCE: Inst. Chemistry, Humboldt Univ., Berlin, Germany
SOURCE: Tetrahedron (1997), 53(1), 185-192
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2-Deoxy-2-C-methylene Me glycosides undergo oxidation with hydrogen peroxide in the presence of molybdenum trioxide as catalyst to afford the corresponding anomeric hydroperoxides. These hydroperoxides were used as chiral oxidants of allylic alcs. and prochiral sulfides to offer moderate enantioselectivities which were, however, higher than those reported before for oxidation with optically active peroxyacids.

RX(1) OF 3



NOTE: enantioselective, key step

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 12 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 122:239362 CASREACT

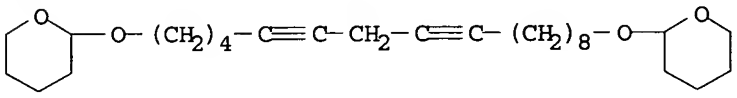
TITLE: A Chemoenzymic Approach to Hydroperoxyeicosatetraenoic Acids. Total Synthesis of 5(S)-HPETE

AUTHOR(S): Dussault, Patrick; Lee, In Quen
CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA

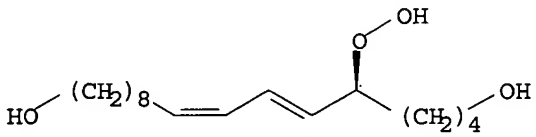
SOURCE: Journal of Organic Chemistry (1995), 60(1), 218-26
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new synthetic approach to enantiomerically pure hydroperoxyeicosatetraenoic acids (HPETEs) is described in which the tetraene skeleton is assembled through chemoselective olefination of a protected hydroperoxy aldehyde. Soybean lipoxygenase-mediated dioxygenation of both natural and unnatural fats produces hydroperoxy dienes in high enantiomeric excess; the observed regioselectivity supports a revised hypothesis for substrate specificity. Protection of the diene hydroperoxides as peroxy ketals is followed by regioselective ozonolysis to afford enantiomerically pure 4-peroxy 2,3-enals which undergo olefination to produce peroxytetraenoates. Removal of the monoperoxy ketal and the Me ester affords enantiomerically pure HPETEs. The generality of the strategy is illustrated with the first chemical synthesis of 5(S)-HPETE, 5(S)-hydroperoxy-(6E,8Z,11Z,14Z)-eicosatetraenoic acid.

RX(146) OF 337 - 3 STEPS



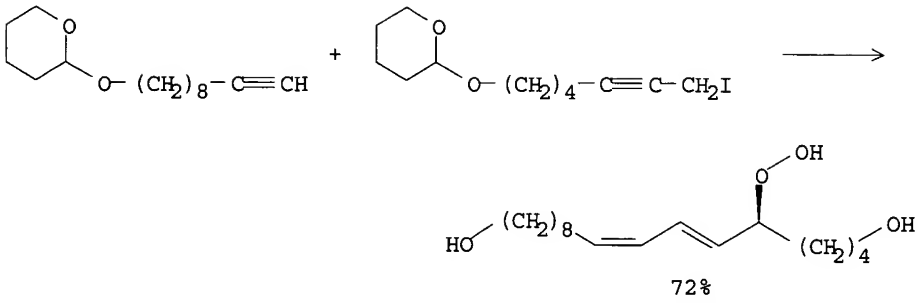
1.1. Ni(OAc)2, H2, NaBH4, EtOH, Water
1.2. H2NCH2CH2NH2, EtOH
2.1. p-MeC6H4SO3H.H20, MeOH
2.2. Na2CO3, Water
3.1. O2, Water, EtOH
3.2. 2,6-Di-t-butylcresol,



72%

NOTE: 1) stereoselective, 3) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

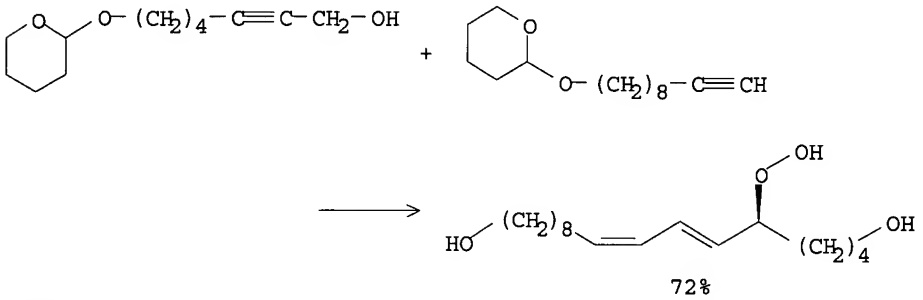
RX(149) OF 337 - 4 STEPS



72%

NOTE: 2) stereoselective, 4) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

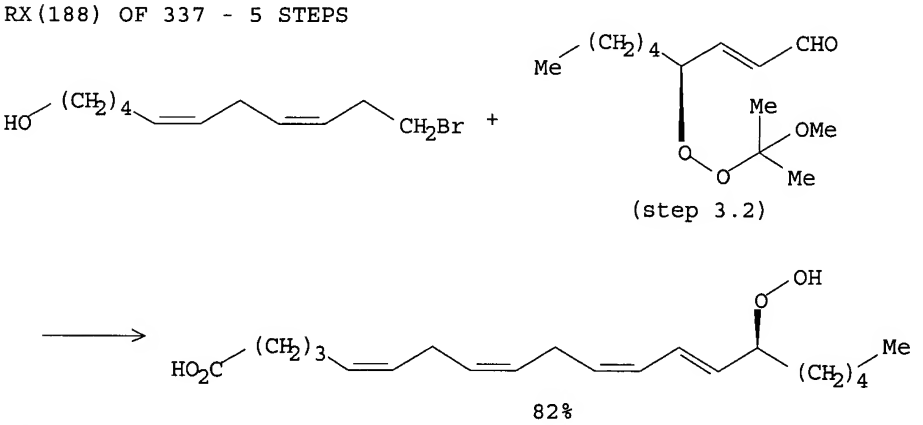
RX(172) OF 337 - 5 STEPS



72%

NOTE: 3) stereoselective, 5) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(188) OF 337 - 5 STEPS

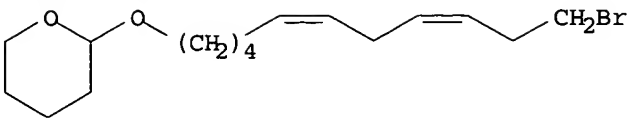


(step 3.2)

82%

NOTE: 2) no exptl. detail, 3) stereoselective, Wittig olefination, key step, 4) safety-peroxides (BHT used), 5) safety-peroxides (BHT used)

RX(190) OF 337 - 6 STEPS



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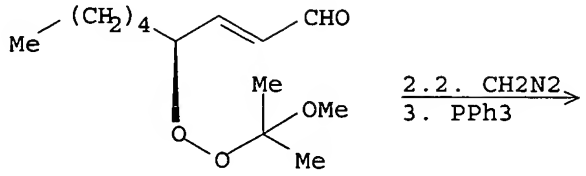
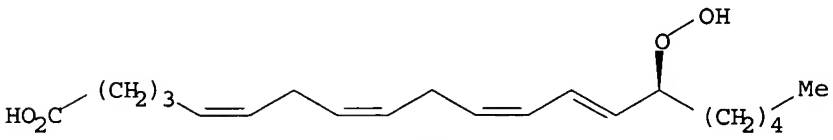


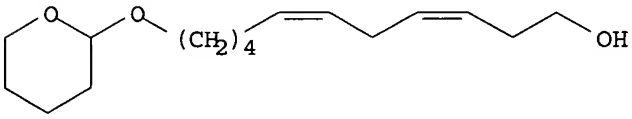
(step 4.2)



82%

NOTE: 3) no exptl. detail, 4) stereoselective, Wittig olefination, key step, 5) safety-peroxides (BHT used), 6) safety-peroxides (BHT used)

RX(192) OF 337 - 7 STEPS



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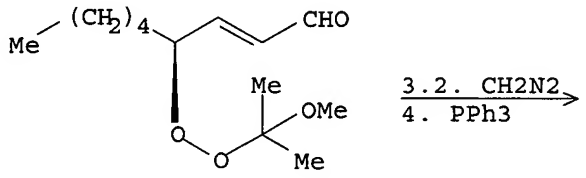
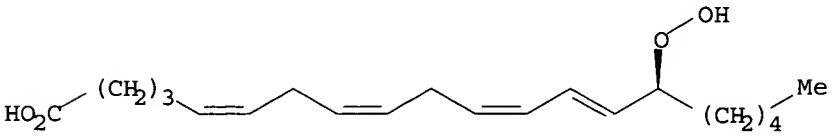


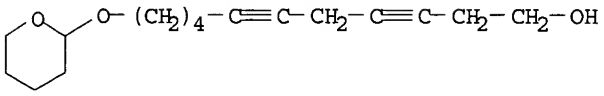
(step 5.2)



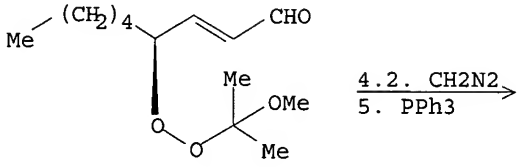
82%

NOTE: 4) no exptl. detail, 5) stereoselective, Wittig olefination, key step, 6) safety-peroxides (BHT used), 7) safety-peroxides (BHT used)

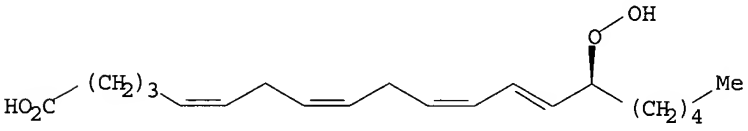
RX(194) OF 337 - 8 STEPS



+



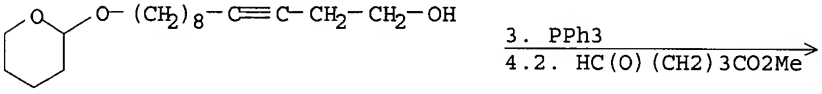
(step 6.2)

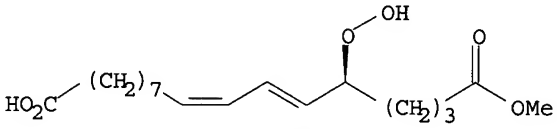


82%

NOTE: 1) stereoselective, 5) no exptl. detail, 6) stereoselective, Wittig olefination, key step, 7) safety-peroxides (BHT used), 8) safety-peroxides (BHT used)

RX(218) OF 337 - 7 STEPS

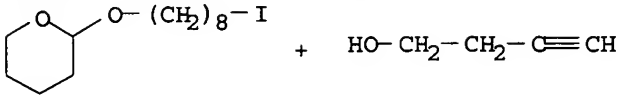




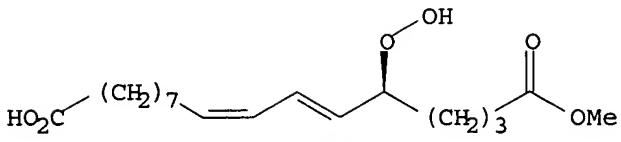
84%

NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(219) OF 337 - 8 STEPS



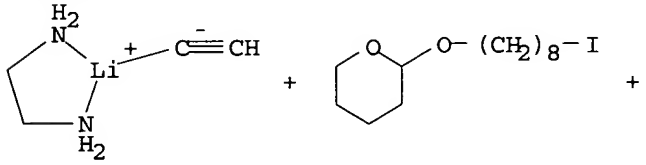
4. PPh3
5.2. HC(O)(CH2)3CO2Me

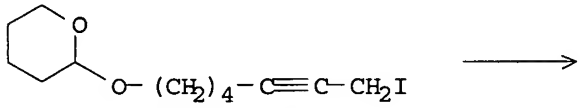


84%

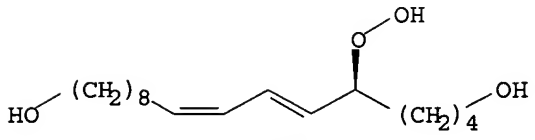
NOTE: 1) regioselective, 2) stereoselective, 5) stereoselective, Wittig olefination, key step, 7) Jones reagent used, 8) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(249) OF 337 - 5 STEPS





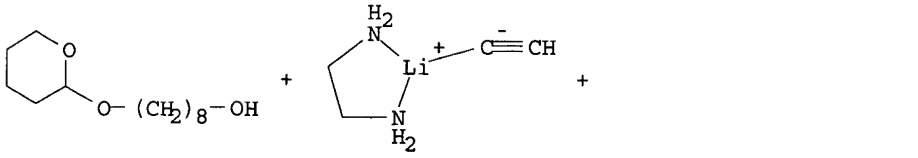
(step 2.3)



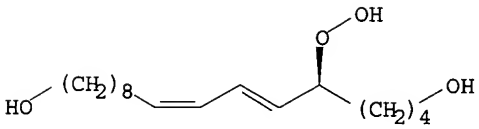
72%

NOTE: 3) stereoselective, 5) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(253) OF 337 - 6 STEPS



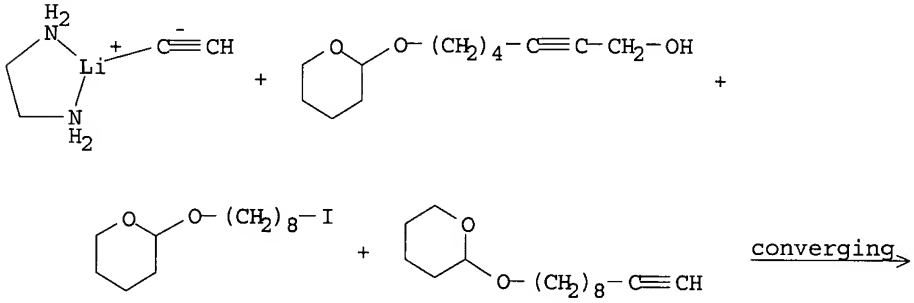
(step 3.3)



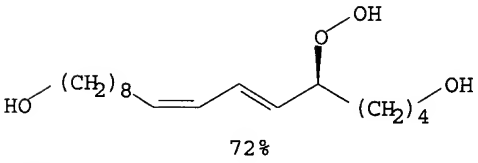
72%

NOTE: 4) stereoselective, 6) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(256) OF 337 - 6 STEPS



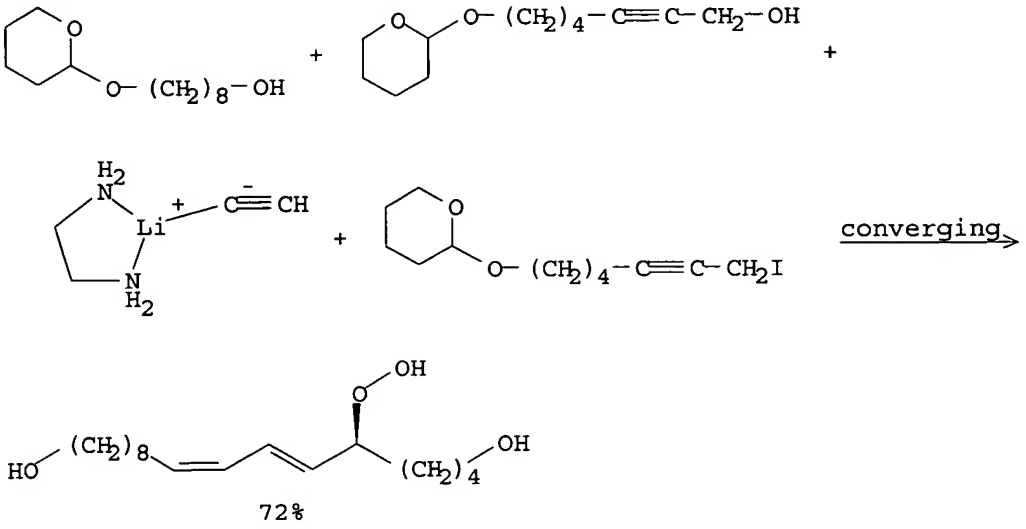
converging



72%

NOTE: stereoselective, stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

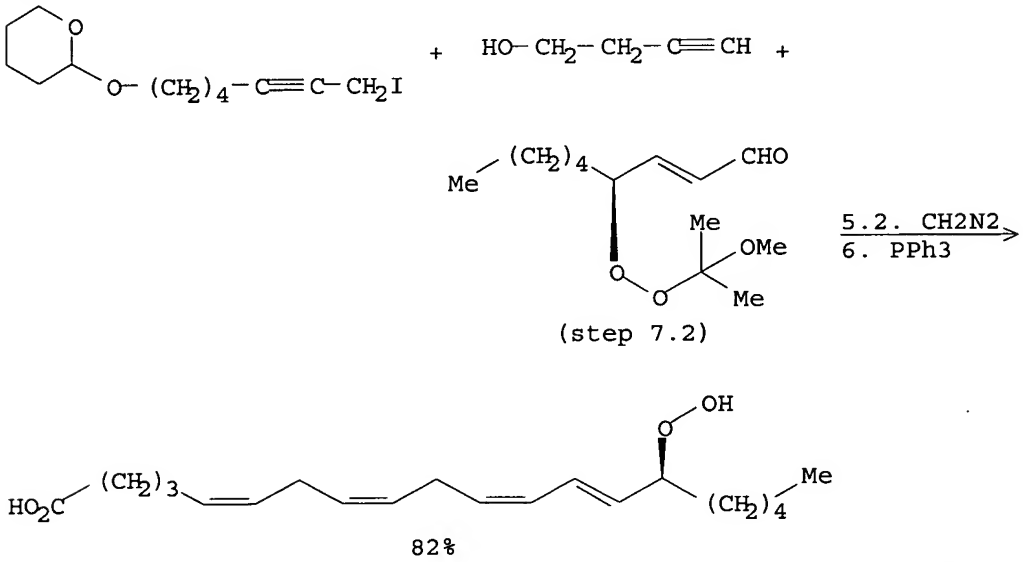
RX(259) OF 337 - 7 STEPS



72%

NOTE: stereoselective, stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(287) OF 337 - 9 STEPS

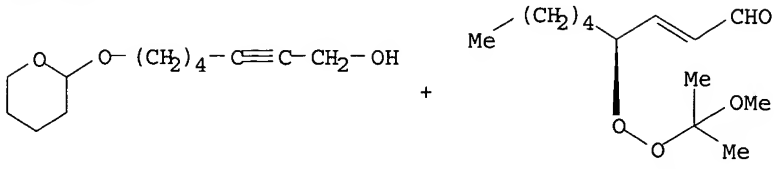


(step 7.2)

82%

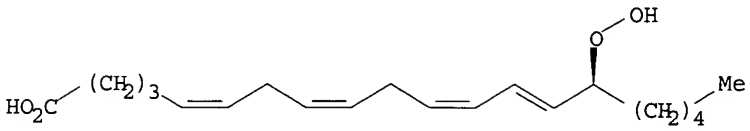
NOTE: 1) regioselective, 2) stereoselective, 6) no exptl. detail, 7) stereoselective, Wittig olefination, key step, 8) safety-peroxides (BHT used), 9) safety-peroxides (BHT used)

RX(289) OF 337 - 10 STEPS



(step 8.2)

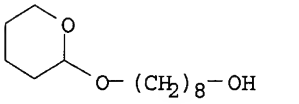
2.1. 3-Butynol
6.2. CH2N2
7. PPh3



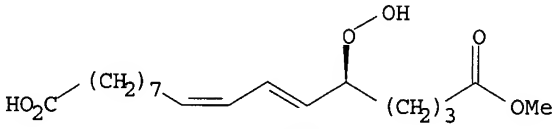
82%

NOTE: 2) regioselective, 3) stereoselective, 7) no exptl. detail, 8) stereoselective, Wittig olefination, key step, 9) safety-peroxides (BHT used), 10) safety-peroxides (BHT used)

RX(290) OF 337 - 9 STEPS



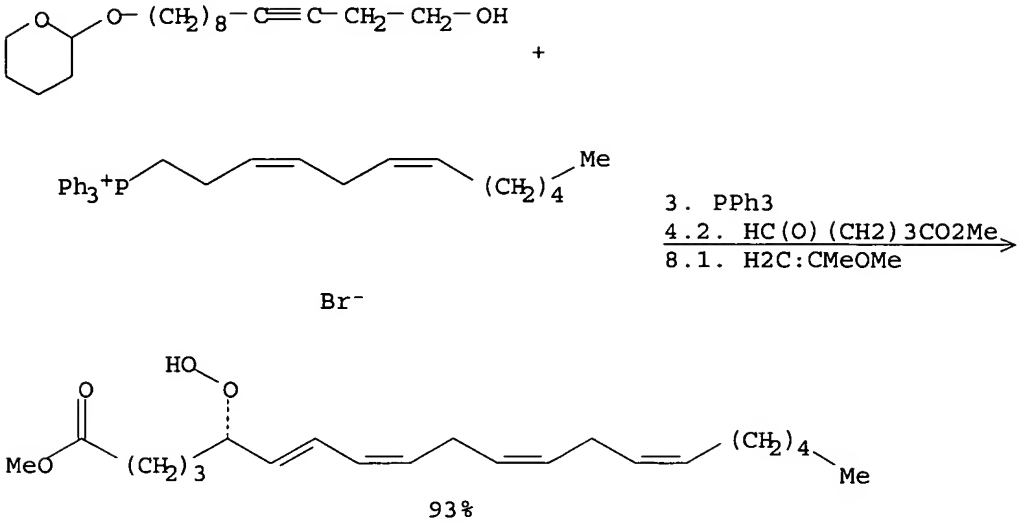
2.1. 3-Butynol
5. PPh3
6.2. HC(O)(CH2)3CO2Me



84%

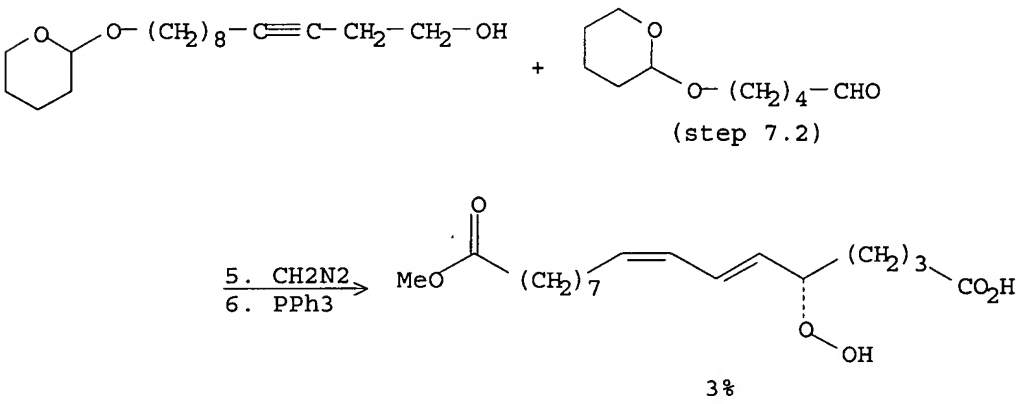
NOTE: 2) regioselective, 3) stereoselective, 6) stereoselective, Wittig olefination, key step, 8) Jones reagent used, 9) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(306) OF 337 - 10 STEPS



NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln., 9) stereoselective, Wittig olefination, key step, 10) safety-peroxides (BHT used)

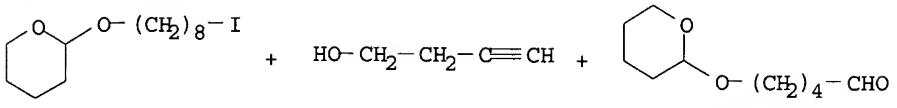
RX(307) OF 337 - 10 STEPS



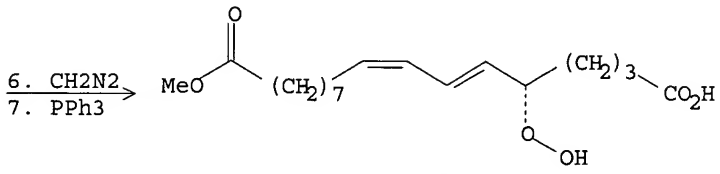
NOTE: 1) stereoselective, 4) Jones reagent used, 7) stereoselective, Wittig olefination, key step, 9) Jones reagent used, 10) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(309) OF 337 - 11 STEPS



(step 8.2)

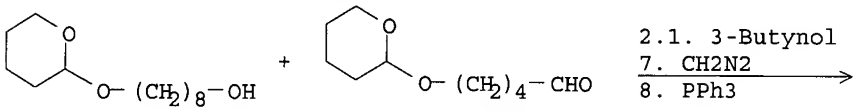


3%

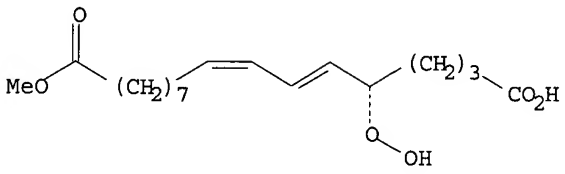
NOTE: 1) regioselective, 2) stereoselective, 5) Jones reagent used, 8) stereoselective, Wittig olefination, key step, 10) Jones reagent used, 11) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(311) OF 337 - 12 STEPS



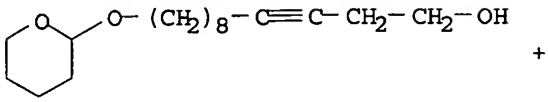
(step 9.2)



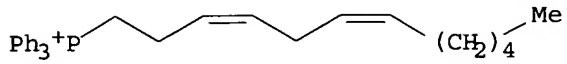
3%

NOTE: 2) regioselective, 3) stereoselective, 6) Jones reagent used, 9) stereoselective, Wittig olefination, key step, 11) Jones reagent used, 12) stereoselective, biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln.

RX(319) OF 337 - 11 STEPS

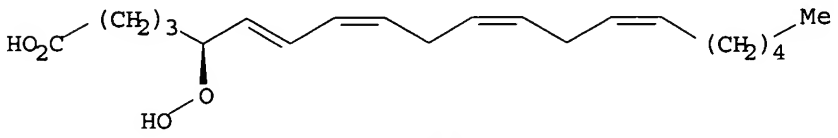


+



3. PPh3
4.2. HC(O)(CH2)3CO2Me
8.1. H2C:CMeOMe

Br-



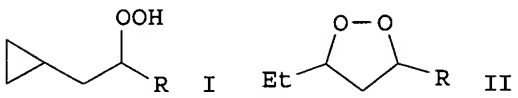
83%

NOTE: 1) stereoselective, 4) stereoselective, Wittig olefination, key step, 6) Jones reagent used, 7) biotransformation, enzymic, soybean type I lipoxygenase used, buffered soln., 9) stereoselective, Wittig olefination, key step, 10) safety-peroxides (BHT used), 11) safety-peroxides (BHT used)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L34 ANSWER 13 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 116:106138 CASREACT
TITLE: Mercury(II)-mediated cyclization of hydroperoxyalkylcyclopropanes: a new route to cyclic peroxides
AUTHOR(S): Bloodworth, A. J.; Korkodilos, Despoina
CORPORATE SOURCE: Chem. Dep., Univ. Coll. London, London, WC1H 0AJ, UK
SOURCE: Tetrahedron Letters (1991), 32(47), 6953-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

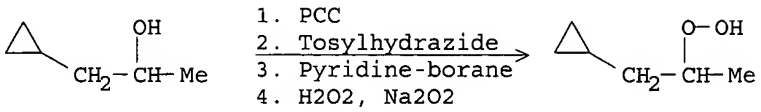


I II

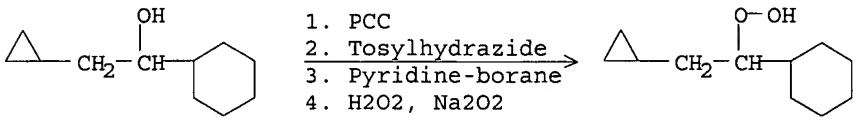
AB Aldehydes, RCHO (R = Me, Et, iso-Pr, cyclohexyl), have been converted via alkylation, cyclopropanation, oxidation, condensation with p-tosylhydrazine, reduction and perhydrolysis into 2-hydroperoxyalkylcyclopropanes I, and thence

by cycloperoxymercuriation and reductive demercuriation into the corresponding 3-alkyl-5-ethyl-1,2-dioxolanes II (R = Me, Et, iso-Pr, cyclohexyl).

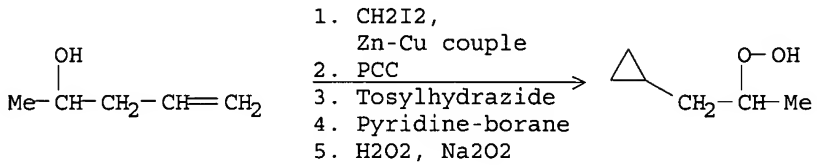
RX(42) OF 72 - 4 STEPS



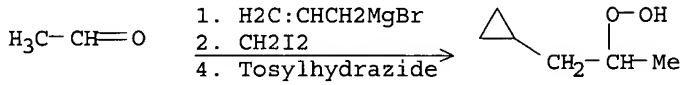
RX(44) OF 72 - 4 STEPS



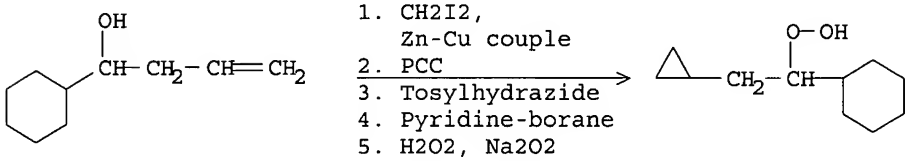
RX(55) OF 72 - 5 STEPS



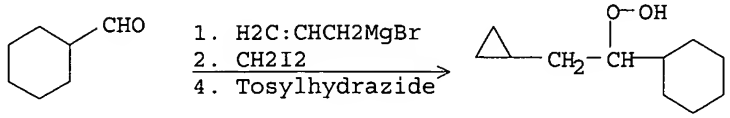
RX(56) OF 72 - 6 STEPS



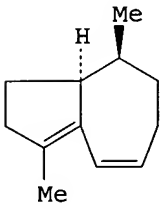
RX(57) OF 72 - 5 STEPS



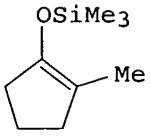
RX(58) OF 72 - 6 STEPS



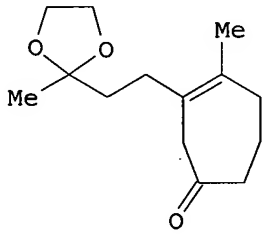
L34 ANSWER 14 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 115:256412 CASREACT
TITLE: Total synthesis of (±)-clavukerin A: a new trinorguaiane sesquiterpene. Biomimetic synthesis of (±)-clavularin A from (±)-clavukerin A
AUTHOR(S): Kim, Sung Kee; Pak, Chwang Siek
CORPORATE SOURCE: Korea Res. Inst. Chem. Technol., Daejeon, S. Korea
SOURCE: Journal of Organic Chemistry (1991), 56(24), 6829-32
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



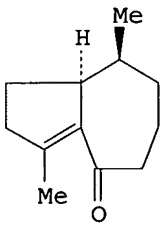
I



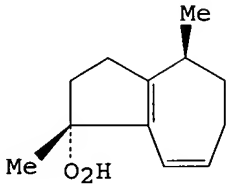
II



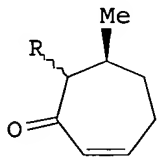
III



IV



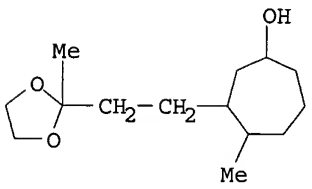
V



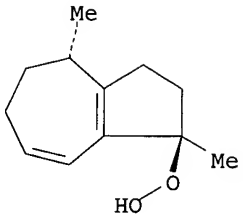
VI

AB (±)-Clavukerin A (I) was synthesized in 8 steps starting from silyl enol ether II in 36% overall yield. The key elements of this synthesis are formation of substituted β,γ-unsatd. cycloheptenone III making using of the previously reported methodol. and highly stereoselective catalytic hydrogenation of III by Rh/alumina followed by acid-catalyzed cyclization to the hydroazulene skeleton IV. The Shapiro reaction was adopted for transformation of enone IV to I. Photooxidn. of I afforded an unstable hydroperoxide, (±)-clavukerin (V), which underwent rearrangement with acid to give (±)-clavularin A and B (VI; R = α-CH2CH2COMe β-CH2CH2COMe; resp). Thus, this methodol. can be utilized as a general method for the preparation of the hydroazulene skeleton.

RX(47) OF 60 - 5 STEPS



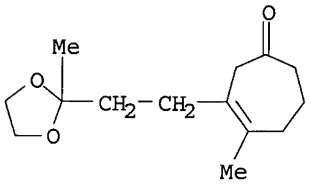
1. PDC, CH2Cl2
2. HCl, EtOH
3. Tosylhydrazide, HCl, MeOH
4. TMEDA, MeLi, THF, Hexane
5. Methylene blue, O2, MeOH, Pyridine



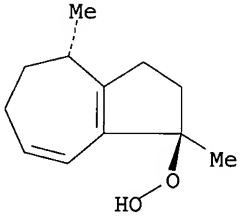
stereoisomers
79%

NOTE: 5) Photochem.

RX(49) OF 60 - 6 STEPS



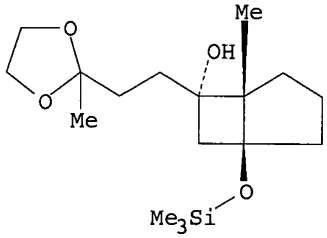
4. Tosylhydrazide



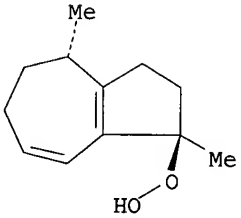
stereoisomers
79%

NOTE: 1) Stereoselective, 6) Photochem.

RX(51) OF 60 - 7 STEPS



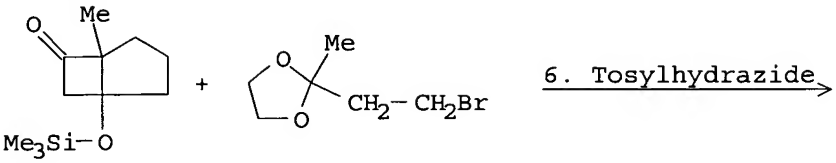
5. Tosylhydrazide

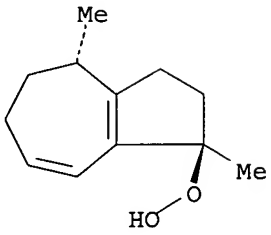


stereoisomers
79%

NOTE: 1) Key step, 2) Stereoselective, 7) Photochem.

RX(52) OF 60 - 8 STEPS





stereoisomers

79%

NOTE: 1) stereoselective, 2) Key step, 3) Stereoselective, 8) Photochem.

L34 ANSWER 15 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 113:212359 CASREACT

TITLE: Stereocontrolled total synthesis of (±)-ptaquilosin, the aglycone of ptaquiloside, a bracken carcinogen

AUTHOR(S): Kigoshi, Hideo; Sawada, Akihiko; Nakayama, Yoshisuke; Niwa, Haruki; Yamada, Kiyoyuki

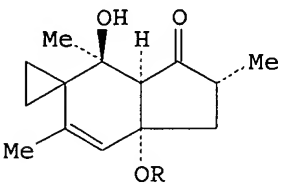
CORPORATE SOURCE: Fac. Sci., Nagoya Univ., Nagoya, 464, Japan

SOURCE: Tetrahedron Letters (1989), 30(15), 1983-6
CODEN: TELEAY; ISSN: 0040-4039

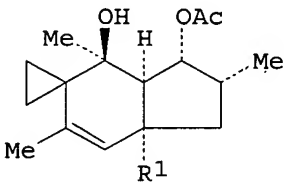
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

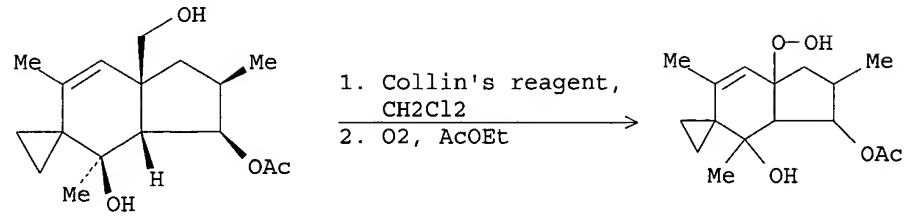


II

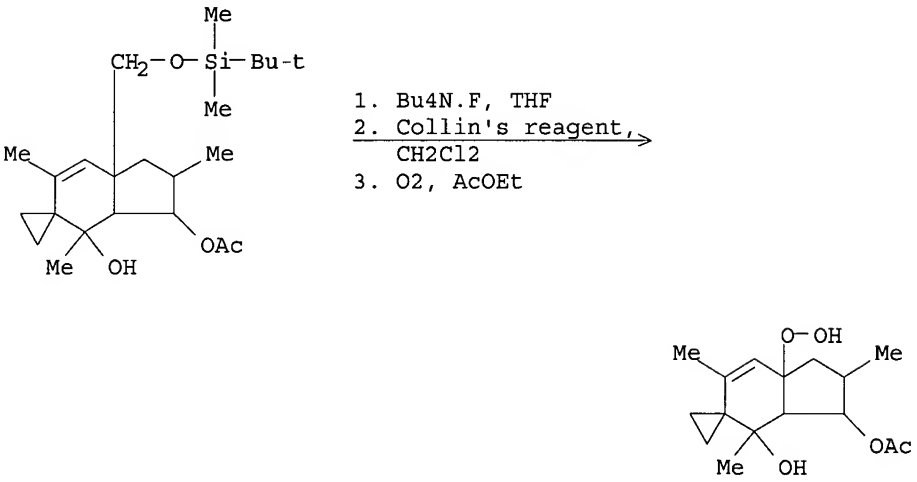
AB Starting from α-allyl-δ-valerolactone, a stereocontrolled synthesis of ptaquilosin (I; R = H), the aglycon of a bracken carcinogen ptaquiloside (I; R = glucosyl) was achieved in racemic form, which includes a novel deformylation-hydroxylation reaction via II (R1 = CHO,

OOH, OH) as one of the key steps.

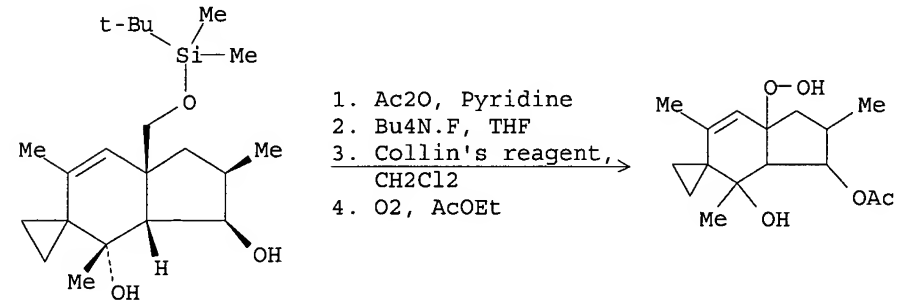
RX(59) OF 592 - 2 STEPS



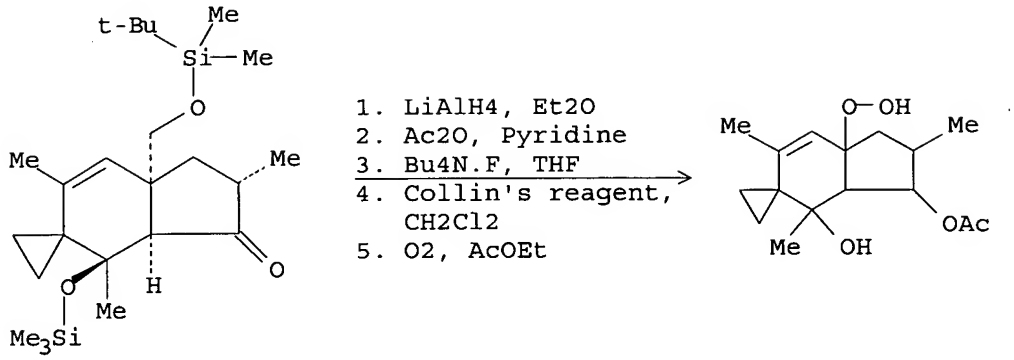
RX(142) OF 592 - 3 STEPS



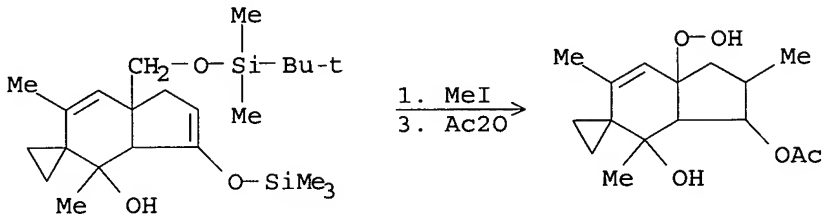
RX(143) OF 592 - 4 STEPS



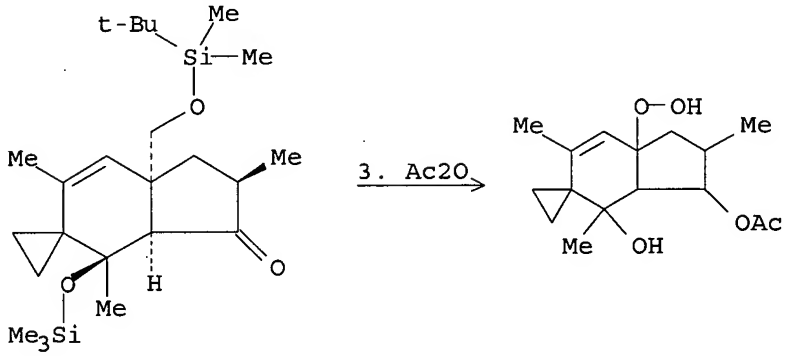
RX(326) OF 592 - 5 STEPS



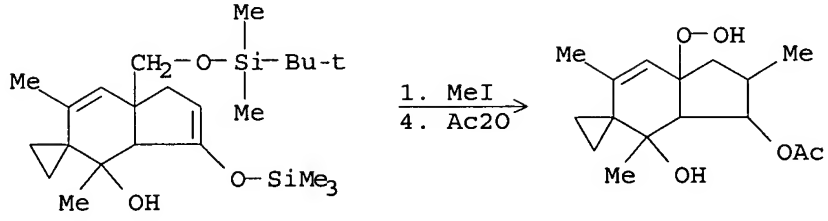
RX(328) OF 592 - 6 STEPS



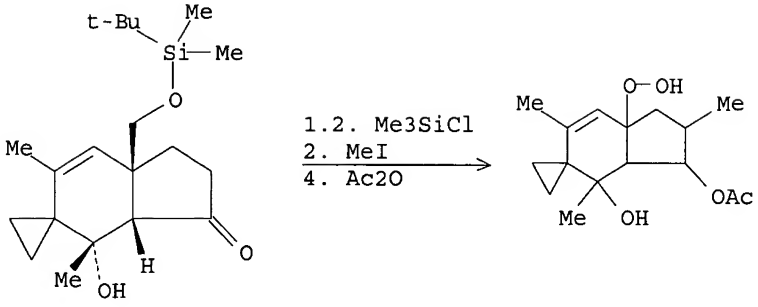
RX(330) OF 592 - 6 STEPS



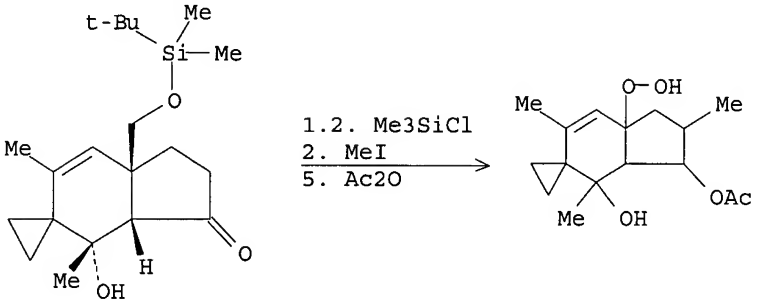
RX(332) OF 592 - 7 STEPS



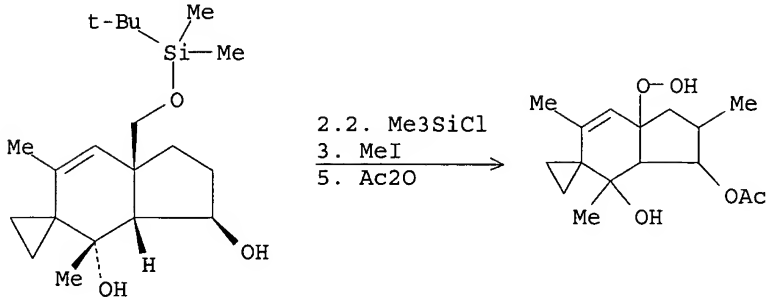
RX(334) OF 592 - 7 STEPS



RX(346) OF 592 - 8 STEPS



RX(347) OF 592 - 8 STEPS



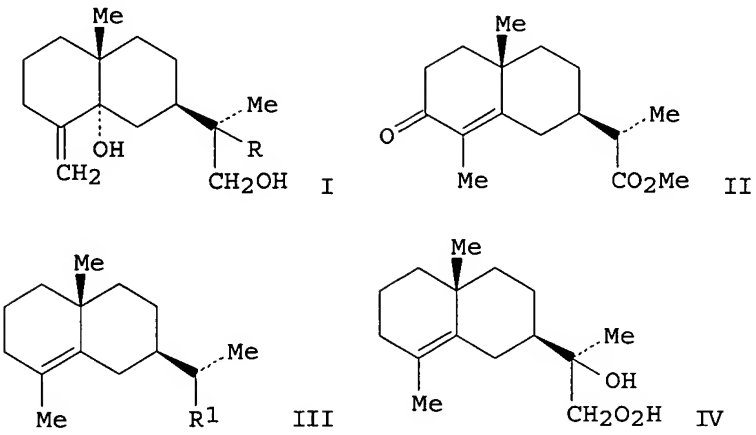
L34 ANSWER 16 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 111:115614 CASREACT
TITLE: Approach to the synthesis of side-chain

eudesmanediols. Synthesis of kudtriol from 1-(α)-santonin

AUTHOR(S): Harapanhalli, Ravi S.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Bombay, 400 076, India

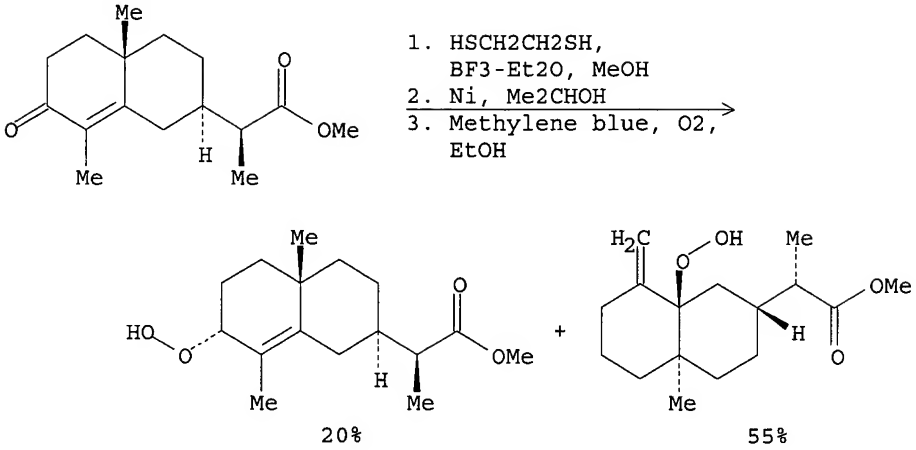
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (12), 3149-54
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



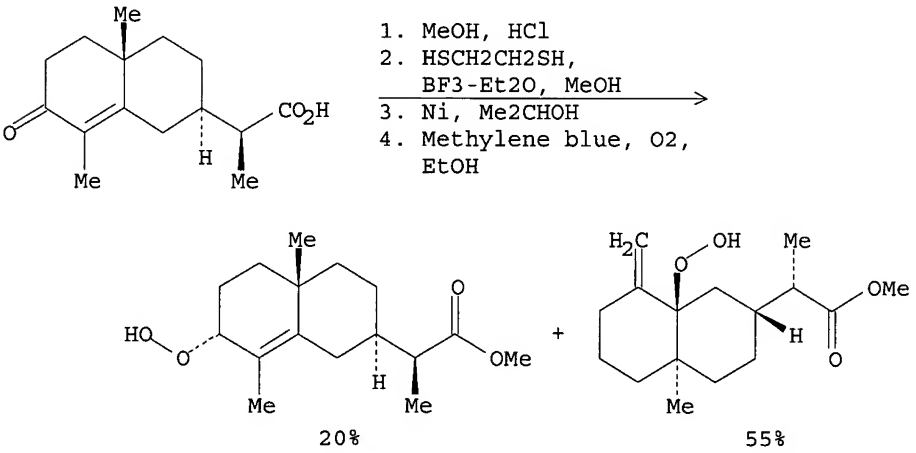
AB Kudtriol (I; R = OH) and its 11-deoxy analog I (R = H) were prepared from 1-(α)-santonin in ten steps. The known intermediate Me (11S)-3-oxoeudesm-4-en-12-oate (II) was taken through the new intermediates Me (11S)-eudesm-4-en-12-oate, (11S)-eudesm-4-en-12-al (III, R1 = CHO), 11-hydroxyeudesm-4-en-12-al, and eudesm-4-ene-11,12-diol (IV). The construction of side-chain diol moiety in IV was achieved by the application of Vedejs' enolate hydroxylation on III (R1 = CHO). The sensitized photooxygenation-reduction sequence transformed IV into I (R = OH). A similar sequence on (11S)-eudesm-4-en-12-ol (III; R1 = CH2OH) resulted in I (R = H).

RX(39) OF 67 - 3 STEPS



NOTE: 3) photochem.

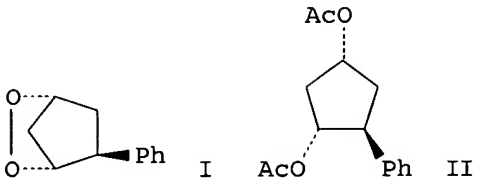
RX(41) OF 67 - 4 STEPS



NOTE: 4) photochem.

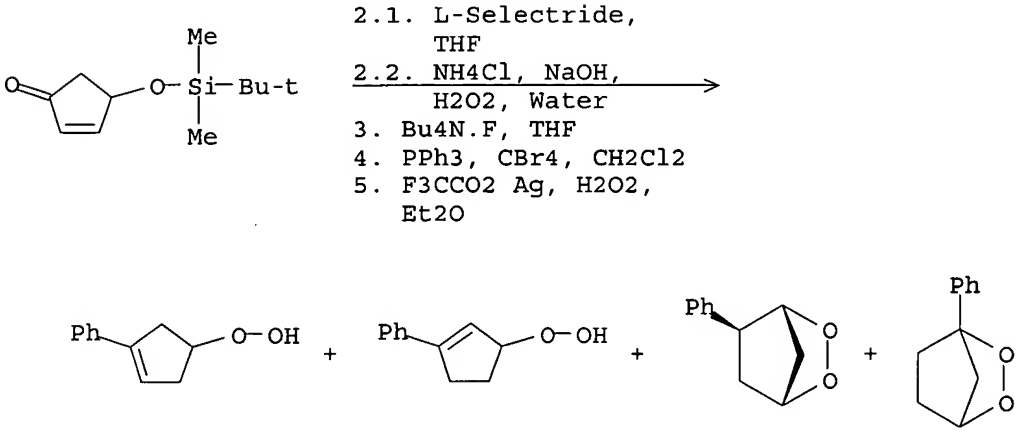
L34 ANSWER 17 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 109:37642 CASREACT
TITLE: Formation of 1-phenyl-2,3-dioxabicyclo[2.2.1]heptane in the reaction of 1,3-dibromo-4-phenylcyclopentane with hydrogen peroxide in the presence of silver trifluoroacetate
AUTHOR(S): Takahashi, Kimio; Shiro, Motoo; Kishi, Morio
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Organic Chemistry (1988), 53(13), 3098-104

CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

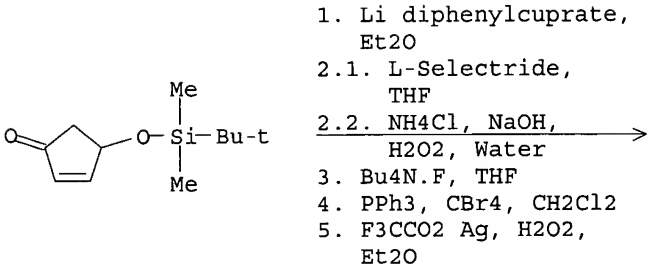


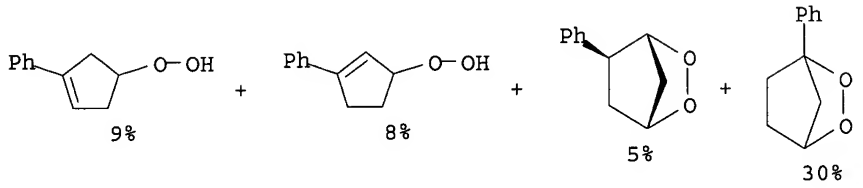
AB Reaction of 1,3-dibromo-4-phenylcyclopentane, prepared from 4-hydroxycyclopent-2-en-1-one in a stereocontrolled manner, or its stereoisomer with anhydrous H2O2 in the presence of CF3CO2Ag gave 1-phenyl-2,3-dioxabicyclo[2.2.1]heptane as the main rearranged product. The expected 5-phenyl-2,3-dioxabicyclo[2.2.1]heptane (I) and phenylcyclopentenyl hydroperoxides were also formed in this reaction. An authentic sample of endoperoxide I was prepared by using peroxide transfer reaction between (Bu3SnO)2 and the bis(triflate) of all-cis-phenylcyclopentanediol. The stereochem. of I and related compds. was confirmed by correlation with the data from x-ray crystallog. anal. of the diacetate II obtained from I by SnCl2 reduction

RX(179) OF 393 - 5 STEPS

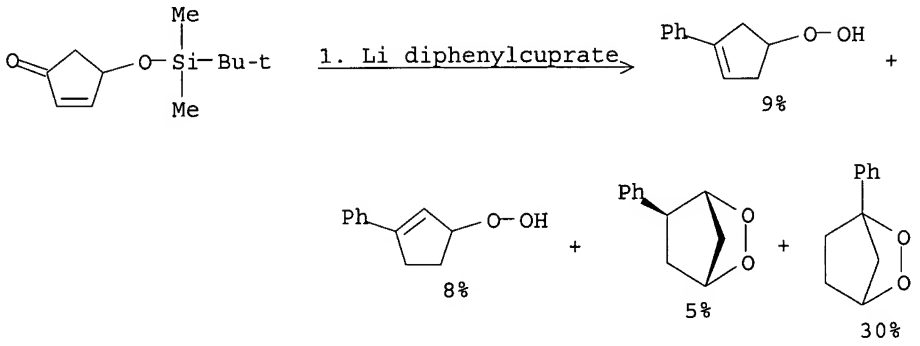


RX(180) OF 393 - 5 STEPS

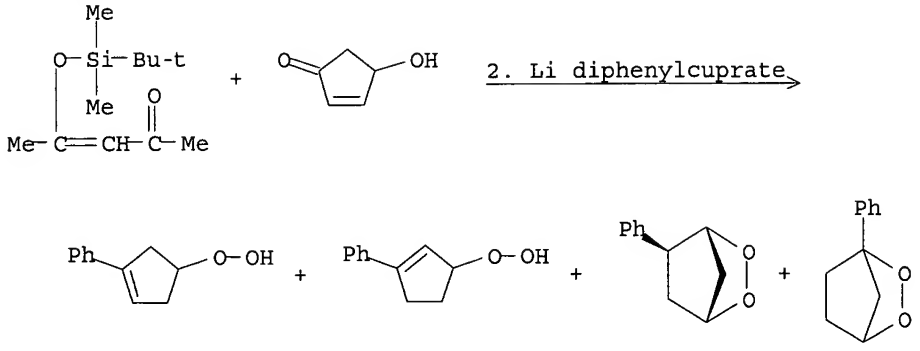




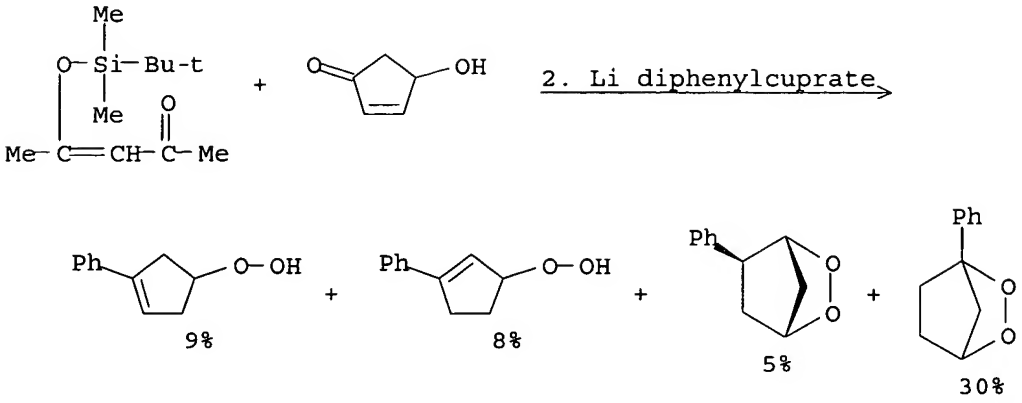
RX(181) OF 393 - 5 STEPS



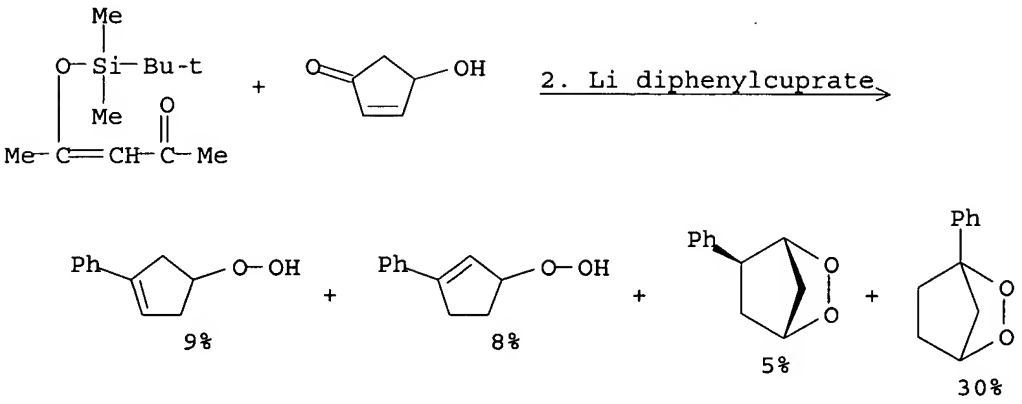
RX(184) OF 393 - 6 STEPS



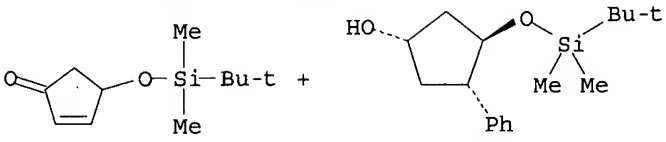
RX(185) OF 393 - 6 STEPS



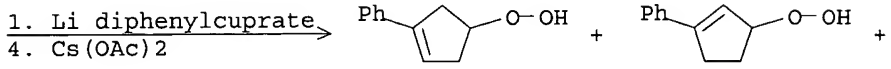
RX(186) OF 393 - 6 STEPS

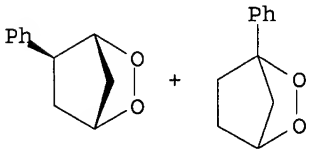


RX(332) OF 393 - 8 STEPS

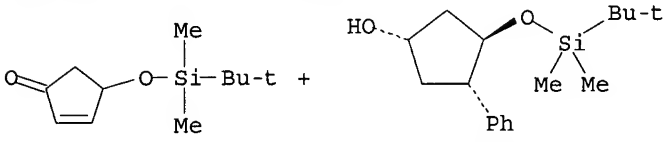


(step 6)

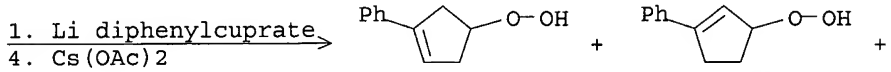




RX(333) OF 393 - 8 STEPS



(step 6)



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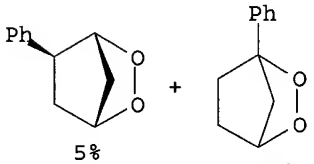
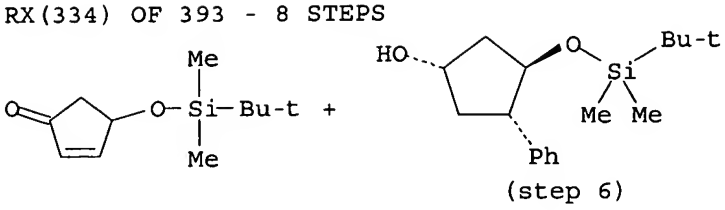
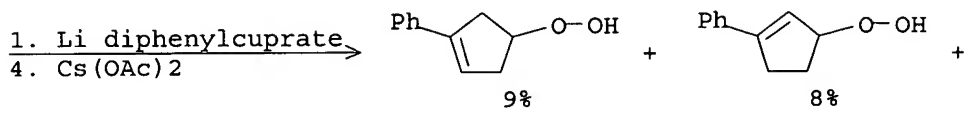


5% 30%

RX(334) OF 393 - 8 STEPS



(step 6)



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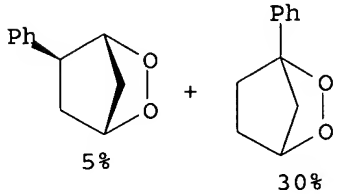
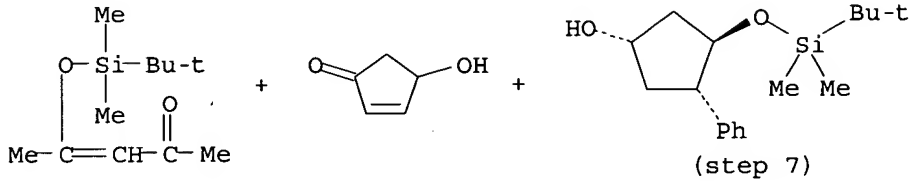


5% 30%

RX(357) OF 393 - 9 STEPS



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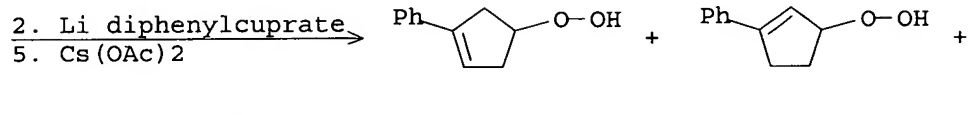
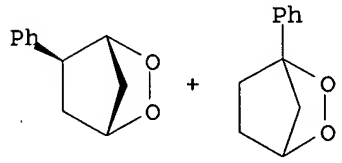
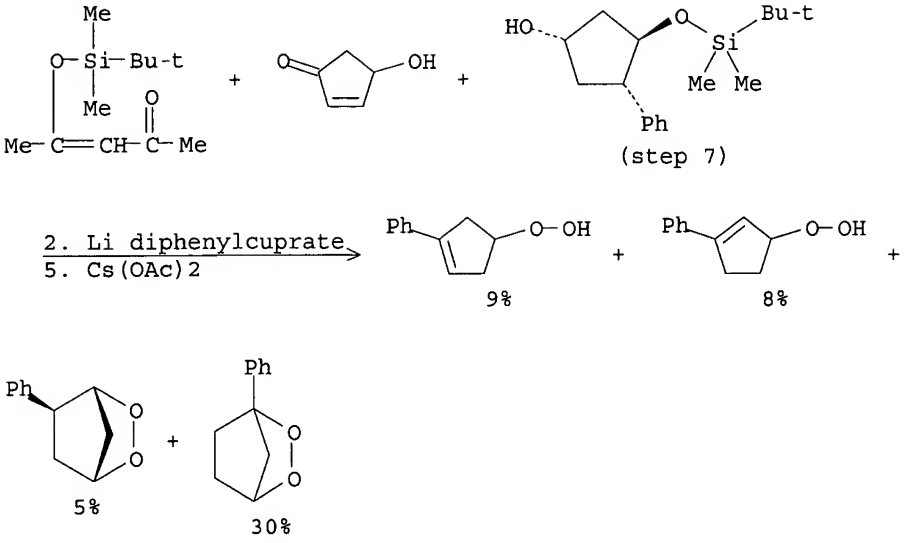
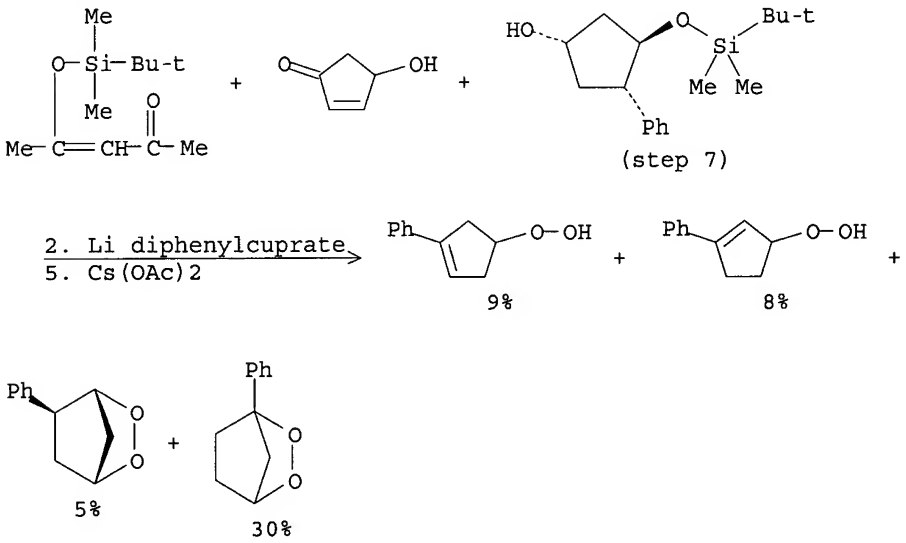




RX(358) OF 393 - 9 STEPS

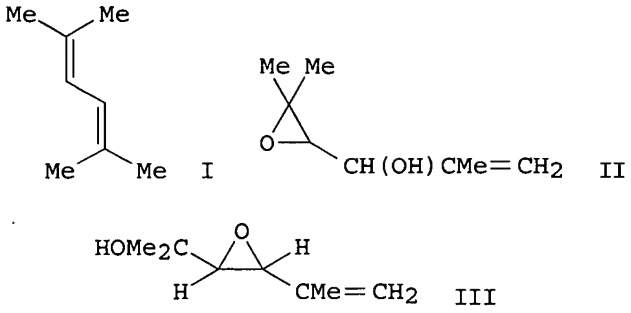


RX(359) OF 393 - 9 STEPS



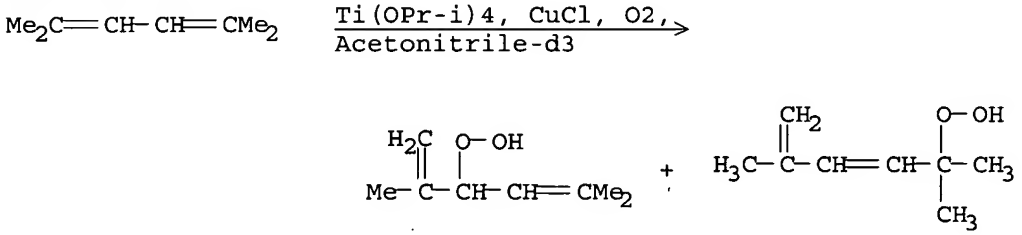
L34 ANSWER 18 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 109:6340 CASREACT
TITLE: Regiocontrolled functionalization of 2,5-dimethyl-2,4-hexadiene into epoxy alcohols by photooxygenation in the presence of titanium(IV) or

vanadium(V)
AUTHOR(S): Adam, Waldemar; Staab, Eugen
CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.
SOURCE: Tetrahedron Letters (1988), 29(5), 531-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Using Ti(OCHMe2)4 as oxygen transfer catalyst, the diene I gave exclusively the epoxy alc. II, whereas the reaction with VO(acac)2 gave exclusively the isomerized epoxy alc. III, via ene reaction with singlet oxygen.

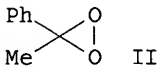
RX(1) OF 16



NOTE: singlet

L34 ANSWER 19 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 110:23463 CASREACT
TITLE: Oxygenation of nitroalkanes with cobalt Schiff base complexes
AUTHOR(S): Nishinaga, Akira; Morikawa, Shohei; Yoshida, Katsumi; Matsuura, Teruo
CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Nippon Kagaku Kaishi (1988), (4), 487-94
CODEN: NKAKB8; ISSN: 0369-4577
DOCUMENT TYPE: Journal

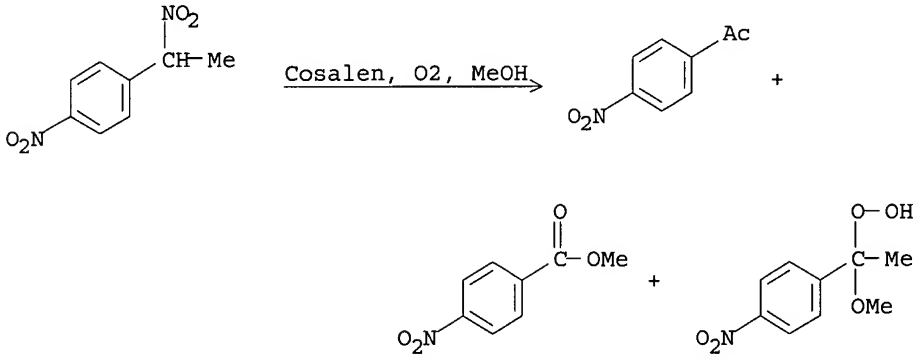
LANGUAGE: Japanese
GI



II

AB Cobalt Schiff base complexes promote the oxygenation of nitroalkanes to give corresponding carbonyl products and (ONO)CoIII(L) (L = Schiff base ligand). The highest selective formation of the carbonyl product with a high conversion is achieved by employing a coordinately saturated hydroxocobalt(III) complex. The oxygenation of PhCHMeNO2 (I) with (HO)CoIII(salen) [salen = (2--OC6H4CH:NCH2)2], a coordinately unsatd. complex, in alcs. gavé the corresponding substituted benzoic acid esters and PhAc. The reaction does not proceed catalytically, because the nitrotocobalt(III) complex formed is inactive. Kinetic studies of the oxygenation of I show that the first step may be an acid-base equilibrium reaction between the substrate and the hydroxo complex giving a substrate anion cobalt(III) complex intermediate. Dioxygen is incorporated into the substrate anion species to give a (1-nitro-1-phenylethylperoxo)cobalt(III) complex, which may decompose to (ONO)CoIII(L) and the dioxirane II, and this dioxane further oxidizes the substrate or the substrate anion species selectively when the peroxocobalt(III) complex is coordinately saturated Otherwise, the peroxo complex in alcs. ROH (R = Me, Et, Me2CH) decomps. to (ONO)COIII(L) and PhCMe(OR)OOH, which undergoes the Baeyer-Villiger decomposition to the benzoic acid esters PhCO2R. A good evidence is available from the oxygenation of 4-O2NC6H4CHMeNO2 with (HO)Co(salen) in MeOH, where 4-O2NC6H4CMe(OMe)OOH is isolated together with 4-O2NC6H4Ac and 4-O2NC6H4CO2Me.

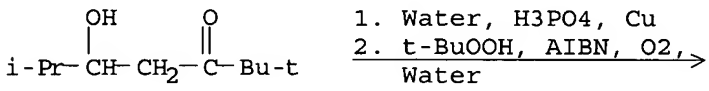
RX(13) OF 15

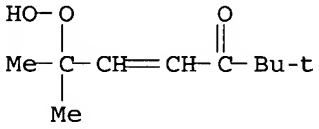


L34 ANSWER 20 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

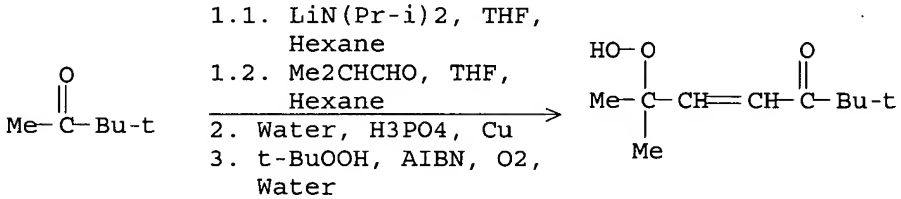
ACCESSION NUMBER: 110:38673 CASREACT
TITLE: γ-Hydroxylation of enones using tert-butyl hydroperoxide and oxygen
AUTHOR(S): Sabol, Mark R.; Wiglesworth, Charlene; Watt, David S.
CORPORATE SOURCE: Lucille Parker Markey Cancer Cent., Univ. Kentucky, Lexington, KY, 40506, USA
SOURCE: Synthetic Communications (1988), 18(1), 1-12
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Free radical hydroxylation of enones, e.g. RCOCH:CHCHR1R1 [I; R = Me3C, R1 = R2 = Me, Et; R = PhMe2C, R1 = R2 = Me; R = PhMe2C, R1R2 = (CH2)7] with Me3COOH-AIBN-O gave 28-68% RCOCH:CHC(OH)R1R2 (II). The yields of II vary as a function of the substitution pattern of the γ-carbon of I. A homolytic mechanism is suggested in which Me3COOH serves as an initiator.

RX(12) OF 14 - 2 STEPS

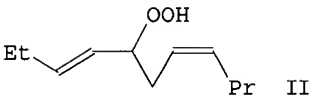




RX(14) OF 14 - 3 STEPS



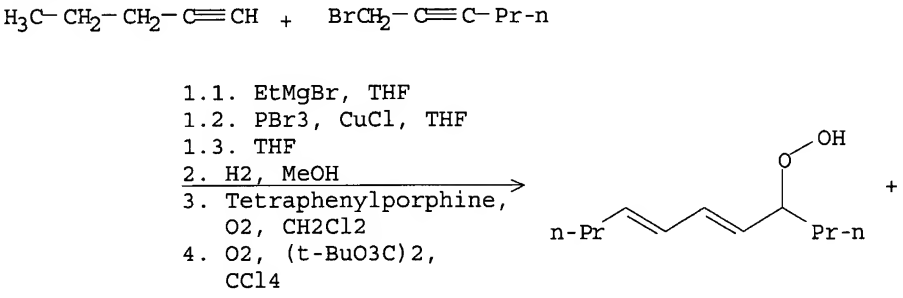
L34 ANSWER 21 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 109:92081 CASREACT
TITLE: Photosensitized oxidation of model unsaturated lipid systems: (4Z,7Z)-undeca-4,7-diene and (4Z)-undec-4-en-7-yne
AUTHOR(S): Carless, Howard A. J.; Batten, Richard J.
CORPORATE SOURCE: Dep. Chem., Birkbeck Coll., London, WC1E 7HX, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (9), 1999-2007
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

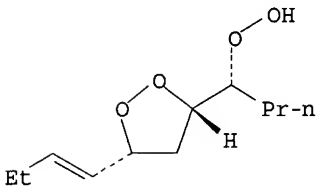


II

AB The photosensitized oxidation of the skipped diene (4Z,7Z)-4,7-undecadiene (I) gave hydroperoxides II and III in a 2:3 ratio. Free radical cyclization of II gave the stereoisomeric dioxolanyl hydroperoxides IV. (4Z)-4-Undecen-7-yne (V) on photosensitized oxidation gave a 1:2 mixture of the nonconjugated and conjugated enynyl hydroperoxides VI and VII. 4,7-Undecadiyne (VIII) was comparatively resistant to photosensitized oxidation; the relative rates of attack on I, V, and VIII are 110:15:≤1. There was no evidence for the abstraction of the 2-propynylic hydrogen by singlet oxygen.

RX(36) OF 65 - 4 STEPS

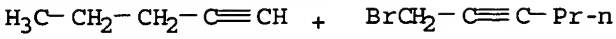


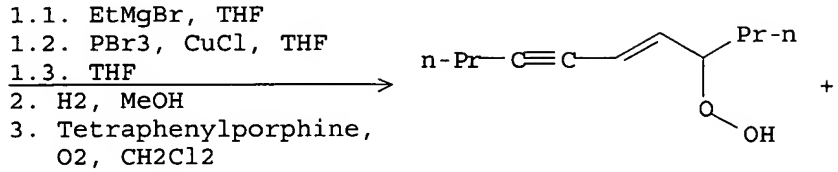


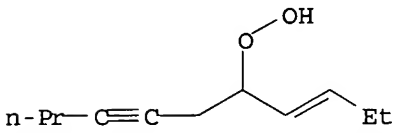
stereoisomers

NOTE: 2) Lindlar catalyst, 3) Photochem.

RX(43) OF 65 - 3 STEPS

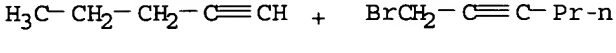


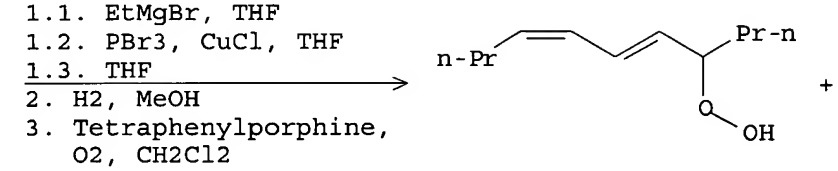


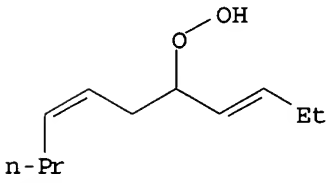


NOTE: 2) Lindlar catalyst, 3) Photochem.

RX(44) OF 65 - 3 STEPS

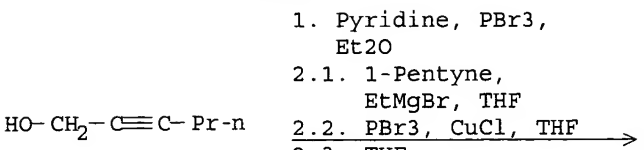


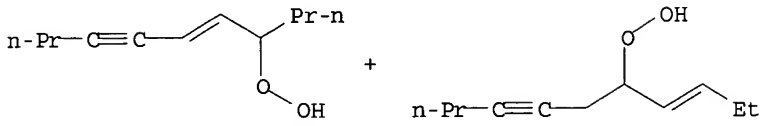




NOTE: 2) Lindlar catalyst, 3) Photochem.

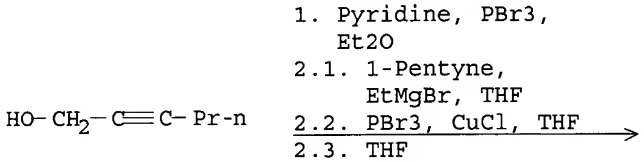
RX(45) OF 65 - 4 STEPS

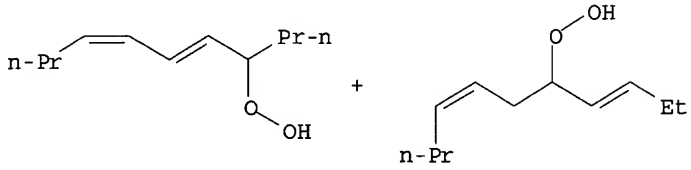




NOTE: 3) Lindlar catalyst, 4) Photochem.

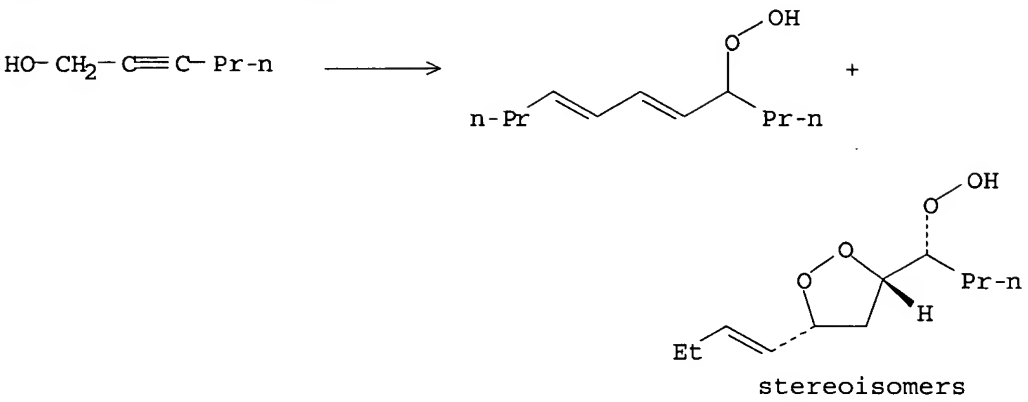
RX(46) OF 65 - 4 STEPS





NOTE: 3) Lindlar catalyst, 4) Photochem.

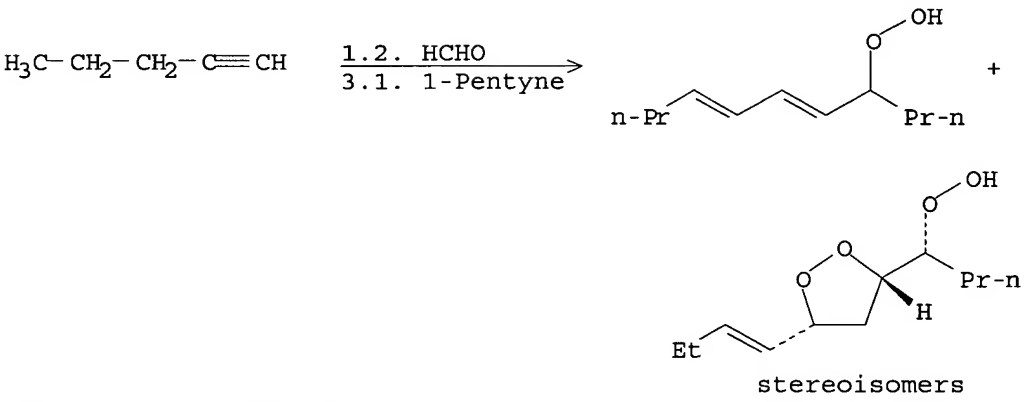
RX(50) OF 65 - 5 STEPS



stereoisomers

NOTE: 3) Lindlar catalyst, 4) Photochem.

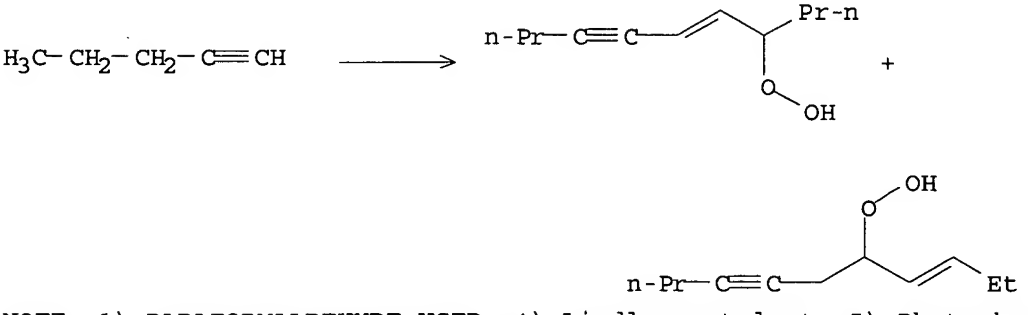
RX(54) OF 65 - 6 STEPS



stereoisomers

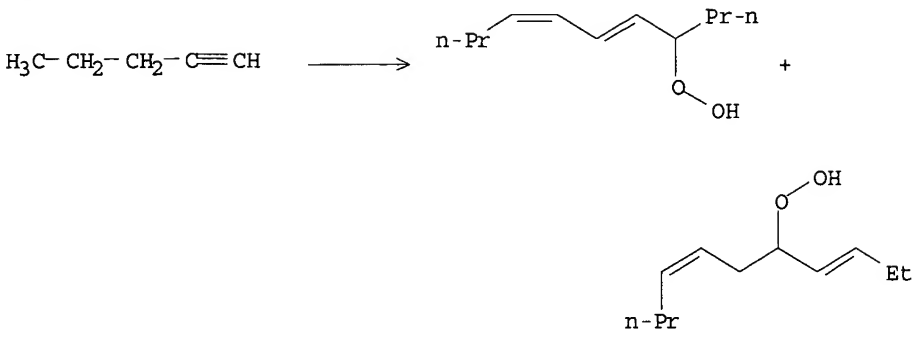
NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

RX(55) OF 65 - 5 STEPS



NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

RX(56) OF 65 - 5 STEPS



NOTE: 1) PARAFORMALDEHYDE USED, 4) Lindlar catalyst, 5) Photochem.

L34 ANSWER 22 OF 76 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 106:5257 CASREACT

TITLE: Practical conversion of artemisinic acid in desoxyartemisinin

AUTHOR(S): Jung, Mankil; ElSohly, Hala N.; Croom, Edward M.; McPhail, Andrew T.; McPhail, Donald R.

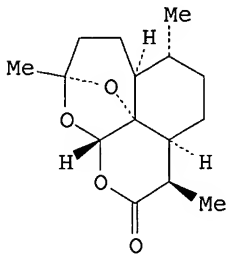
CORPORATE SOURCE: Sch. Pharm., Univ. Mississippi, University, MS, 38677, USA

SOURCE: Journal of Organic Chemistry (1986), 51(26), 5417-19
CODEN: JOCEAH; ISSN: 0022-3263

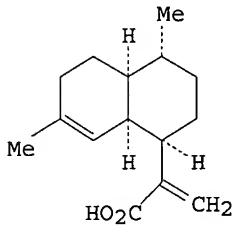
DOCUMENT TYPE: Journal

LANGUAGE: English

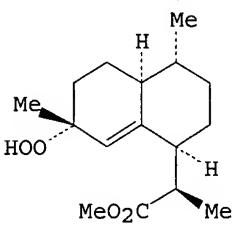
GI



I



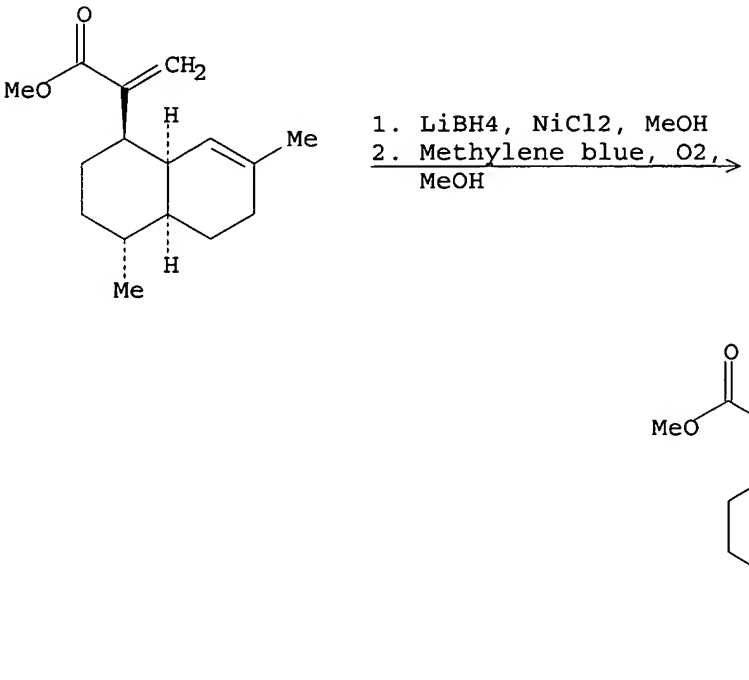
II



III

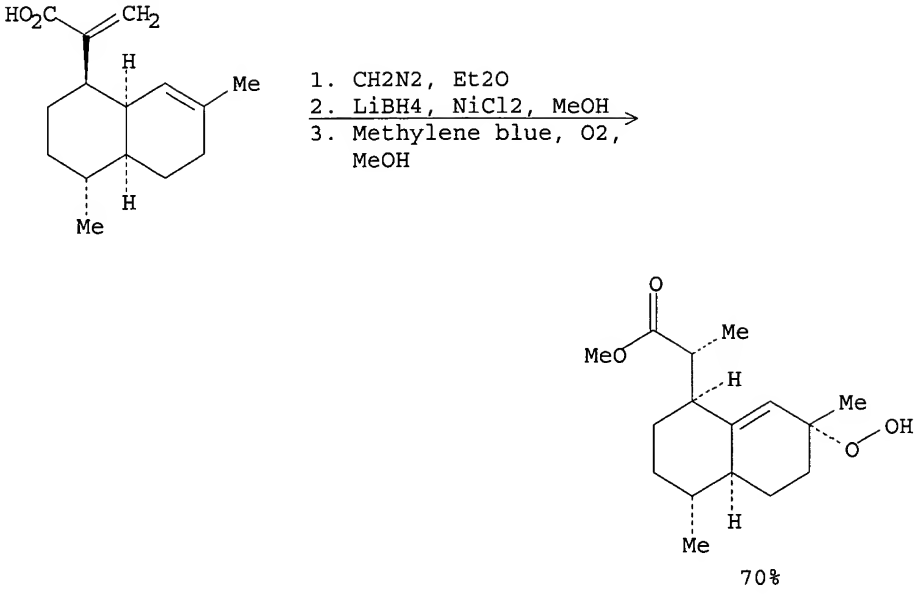
AB Deoxyartemisinin (I) was prepared from artemisinic acid (II) via allylic hydroperoxide III. The structure and absolute configuration of I were confirmed by x-ray crystallog.

RX(7) OF 11 - 2 STEPS



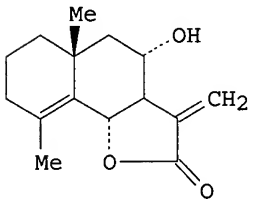
70%

RX(9) OF 11 - 3 STEPS

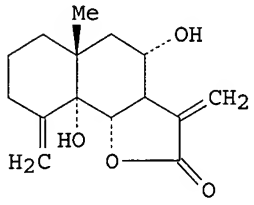


70%

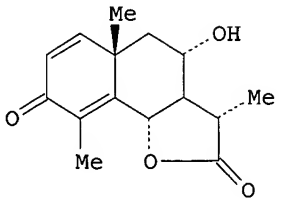
L34 ANSWER 23 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 107:23517 CASREACT
TITLE: Total syntheses of rothin-A and rothin-B
AUTHOR(S): Carda, Miguel; Arno, Manuel; Marco, J. Alberto
CORPORATE SOURCE: Dep. Quim. Org., Fac. Quim., Valencia, Spain
SOURCE: Tetrahedron (1986), 42(13), 3655-62
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



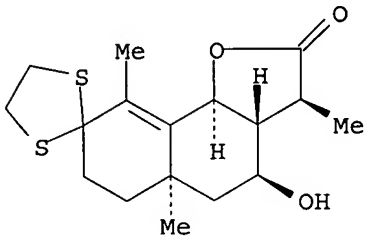
II



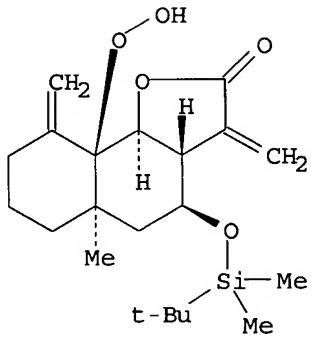
III

AB The eudesmanolides rothin A (I) and rothin B (II) have been synthesized from (-)-artemisin (III) in 7 and 9 steps, resp.

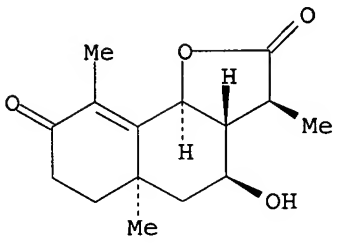
RX(63) OF 99 - 5 STEPS



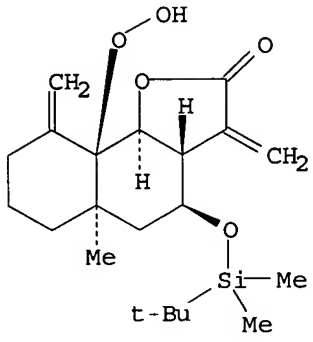
1. Ni
2. t-BuSiMe2Cl, 1H-Imidazole, DMF
3. PhSeCl, LiN(Pr-i)2, Hexane
4. H2O2, AcOH
5. Methylene blue, EtOH



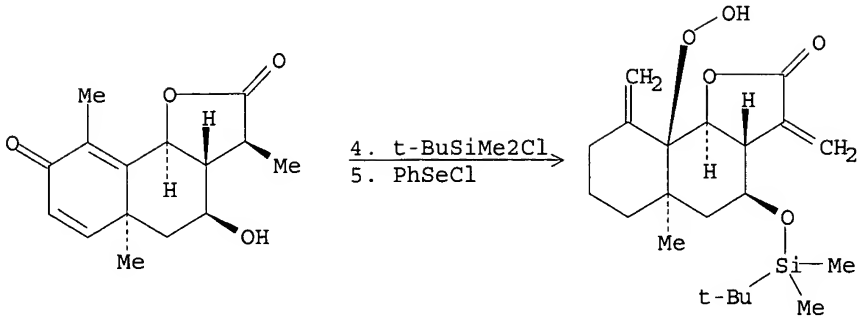
RX(70) OF 99 - 6 STEPS



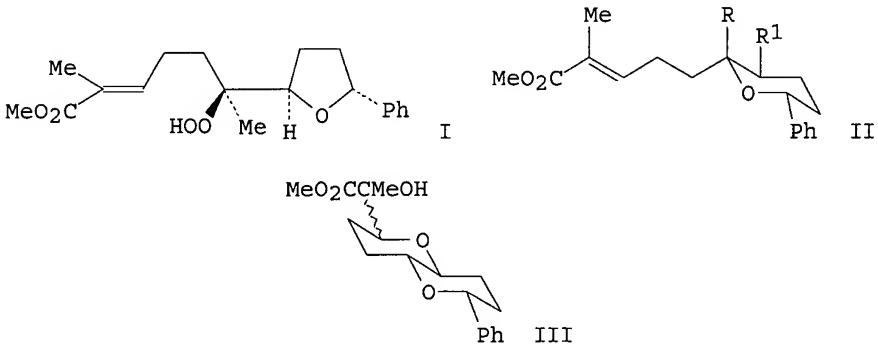
3. t-BuSiMe2Cl
4. PhSeCl



RX(77) OF 99 - 7 STEPS



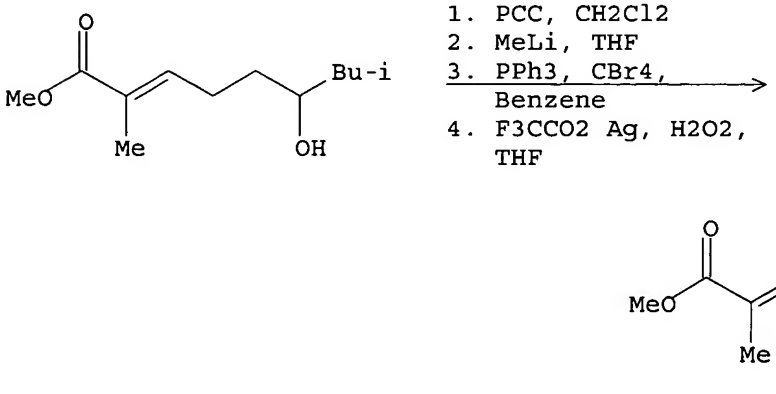
L34 ANSWER 24 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 105:114794 CASREACT
TITLE: Synthesis of polyether-type tetrahydrofurans via hydroperoxide cyclization
AUTHOR(S): Bartlett, Paul A.; Chapuis, Christian
CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Journal of Organic Chemistry (1986), 51(14), 2799-806
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



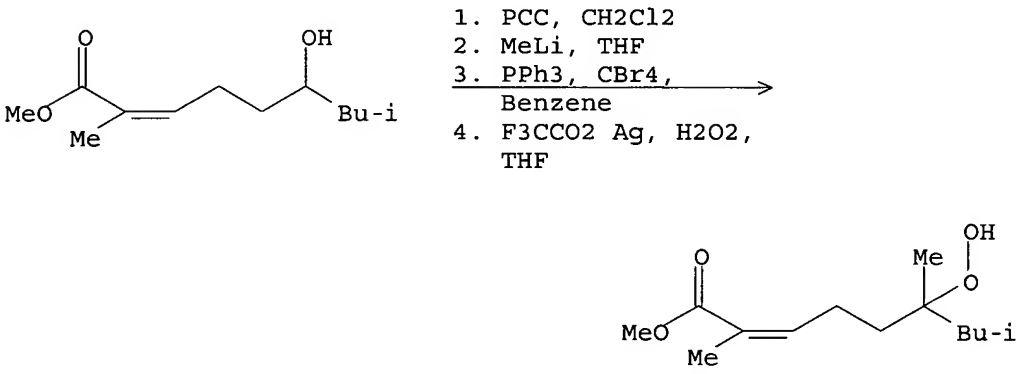
AB Isomerization of an unsatd. hydroperoxy ester to the epoxy alc. and then to the THF was investigated as a method for the stereocontrolled construction of ethers with a substitution pattern appropriate for polyether synthesis. This sequence is highly stereoselective in the case of secondary hydroperoxides, such as MeO2CCMe:CHCH2CH2CHPhOOH, both with respect to the THF stereochem. and the acyclic relationship. With tertiary hydroperoxides, such as MeO2CCMe:CHCH2CH2CRMeOOH (R = Ph, CH2CHMe2), little stereocontrol is seen over the ring stereochem. In the case of the hydroperoxide I, for example, the trans,cis and trans,trans bis ethers are formed in a 1.4:1 ratio. I was prepared stereospecifically from the pyran II (R = Me, R = Br) by a ring contraction process; however,

when this method was applied to II (R = H, R1 = iodo), II (R = H, R1 = OOH) was the major product. Cyclization of II (R = H, R1 = OOH) gave a mixture of the fused bis ethers III.

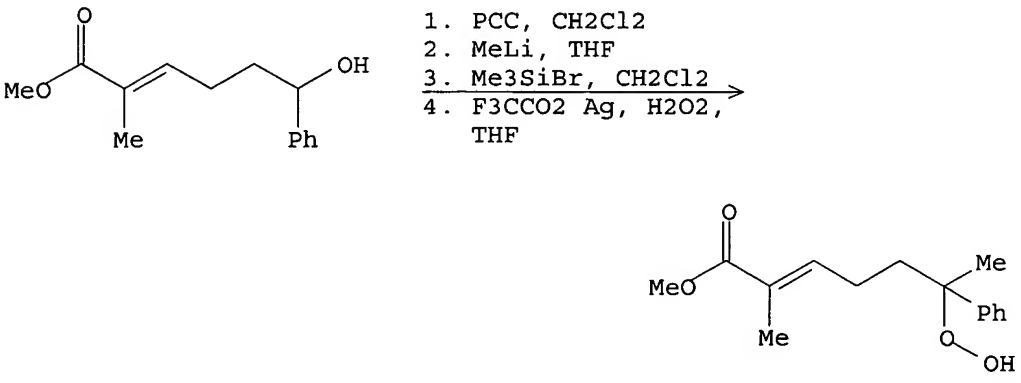
RX(205) OF 707 - 4 STEPS



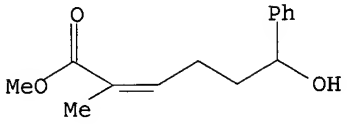
RX(227) OF 707 - 4 STEPS



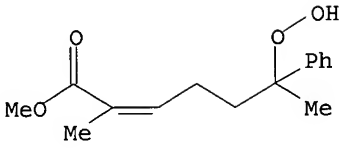
RX(280) OF 707 - 4 STEPS



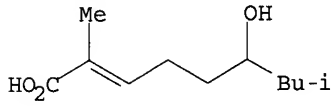
RX(288) OF 707 - 4 STEPS



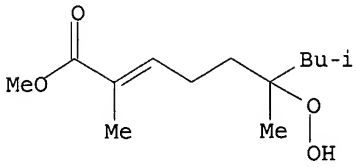
1. PCC, CH2Cl2
2. MeLi, THF
3. Me3SiBr, CH2Cl2
4. F3CCO2 Ag, H2O2, THF



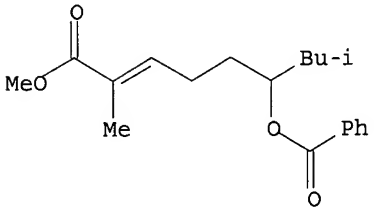
RX(358) OF 707 - 5 STEPS



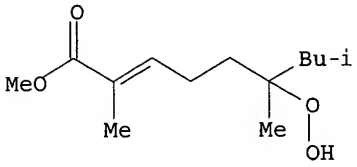
1. CH2N2, Et2O
2. PCC, CH2Cl2
3. MeLi, THF
4. PPh3, CBr4, Benzene
5. F3CCO2 Ag, H2O2, THF



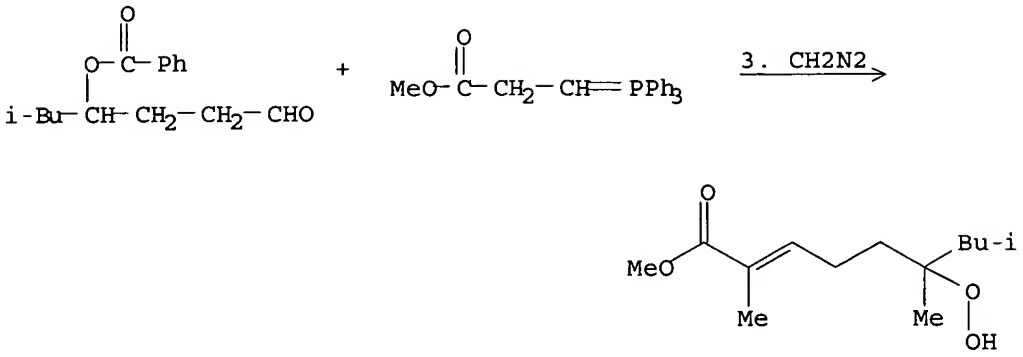
RX(360) OF 707 - 6 STEPS



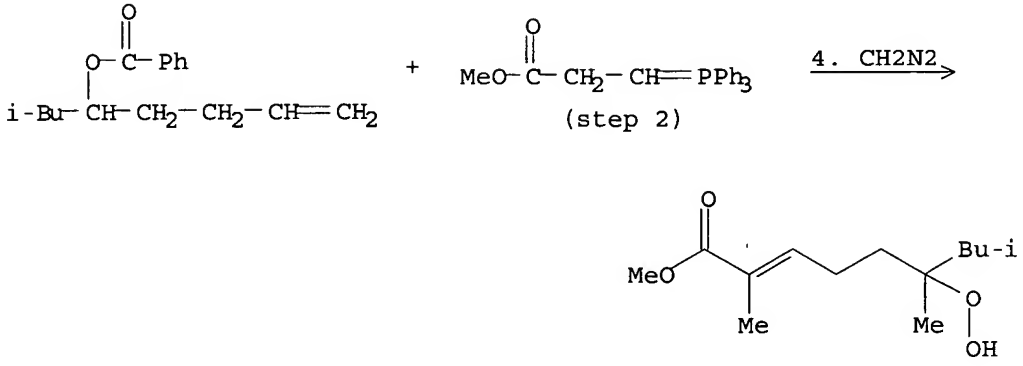
2. CH2N2



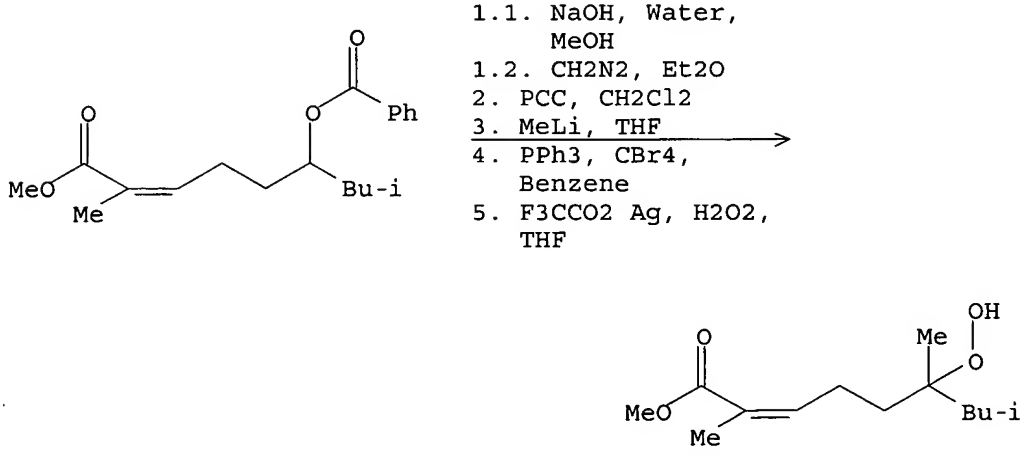
RX(362) OF 707 - 7 STEPS



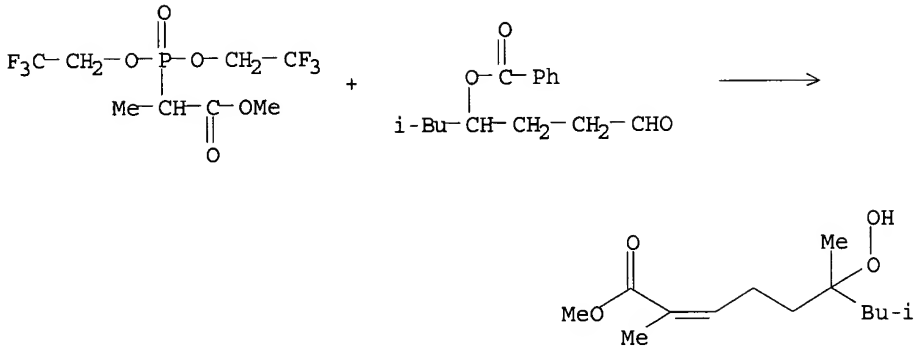
RX(364) OF 707 - 8 STEPS



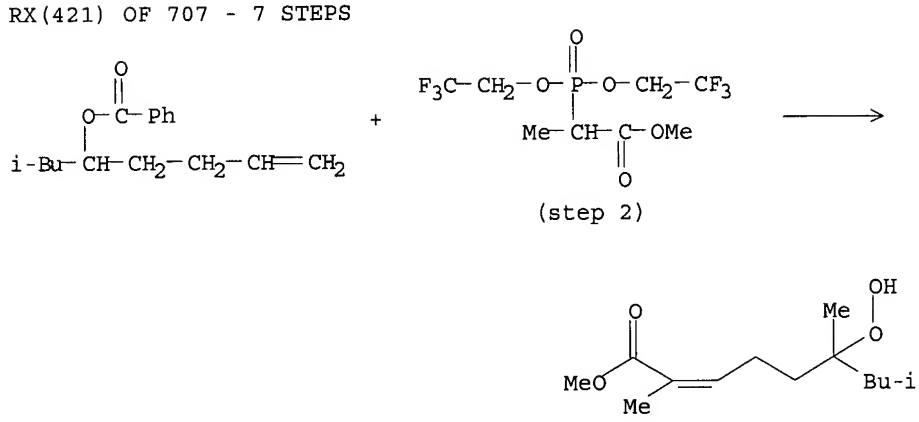
RX(417) OF 707 - 5 STEPS



RX(419) OF 707 - 6 STEPS

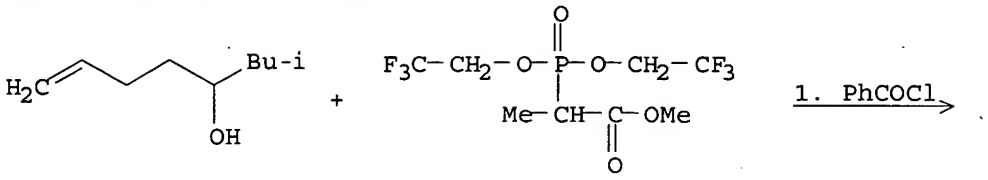


RX(421) OF 707 - 7 STEPS

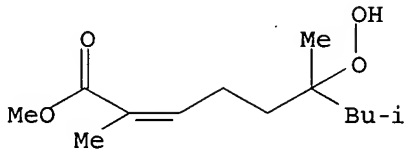


(step 2)

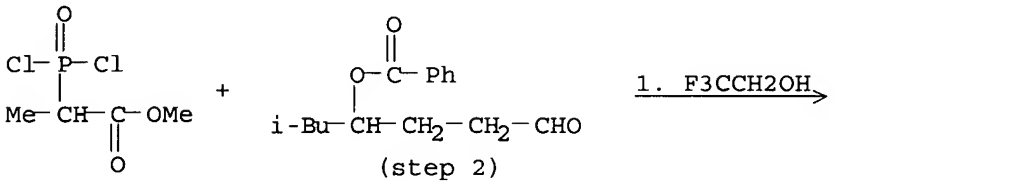
RX(423) OF 707 - 8 STEPS



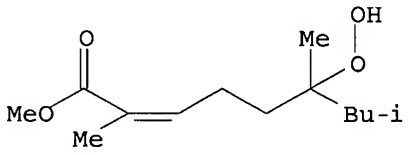
(step 3)



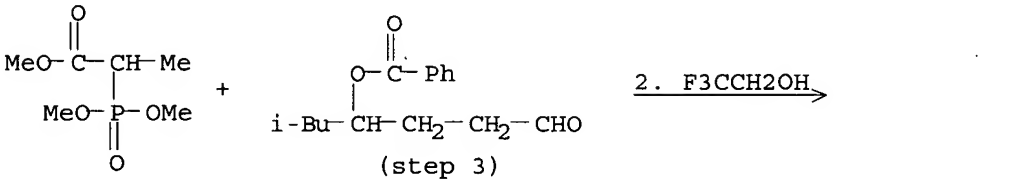
RX(425) OF 707 - 7 STEPS



(step 2)



RX(427) OF 707 - 8 STEPS



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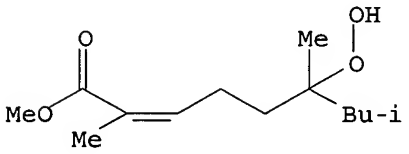
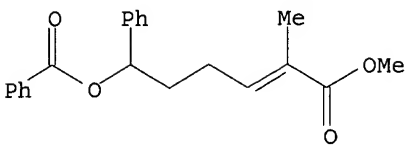
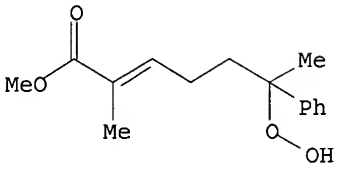


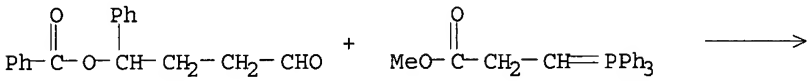
RX(498) OF 707 - 5 STEPS

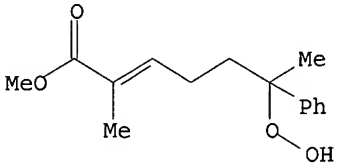


1. NaOH, Water, MeOH
2. PCC, CH2Cl2
3. MeLi, THF
4. Me3SiBr, CH2Cl2
5. F3CCO2 Ag, H2O2, THF

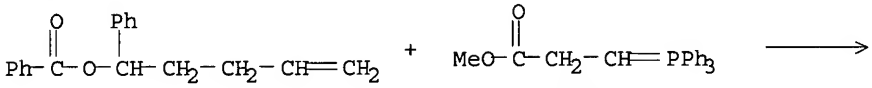


RX(500) OF 707 - 6 STEPS





RX(502) OF 707 - 7 STEPS



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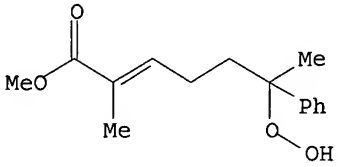
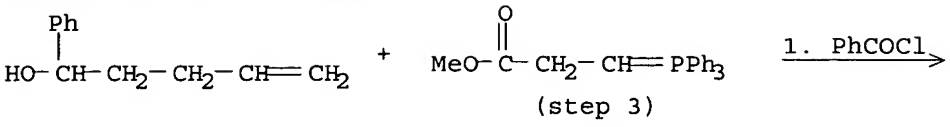
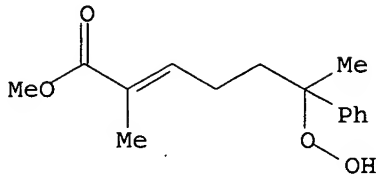
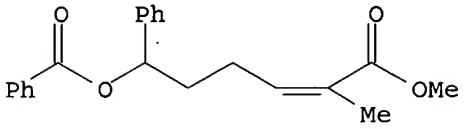


RX(504) OF 707 - 8 STEPS

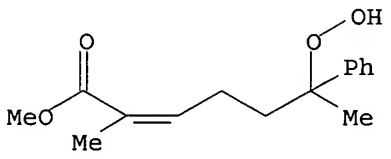




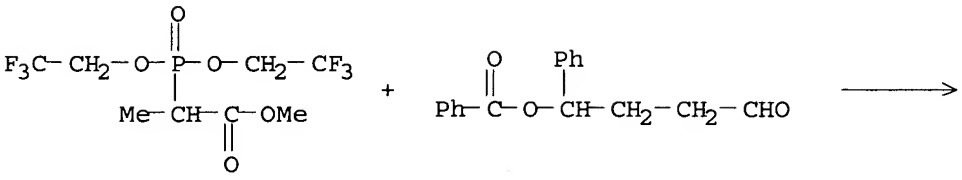
RX(542) OF 707 - 5 STEPS

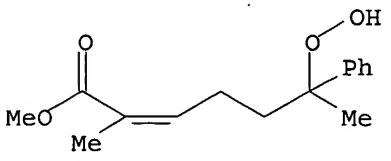


1.1. NaOH, Water, MeOH
1.2. CH2N2, Et2O
2. PCC, CH2Cl2
3. MeLi, THF
4. Me3SiBr, CH2Cl2
5. F3CCO2 Ag, H2O2, THF

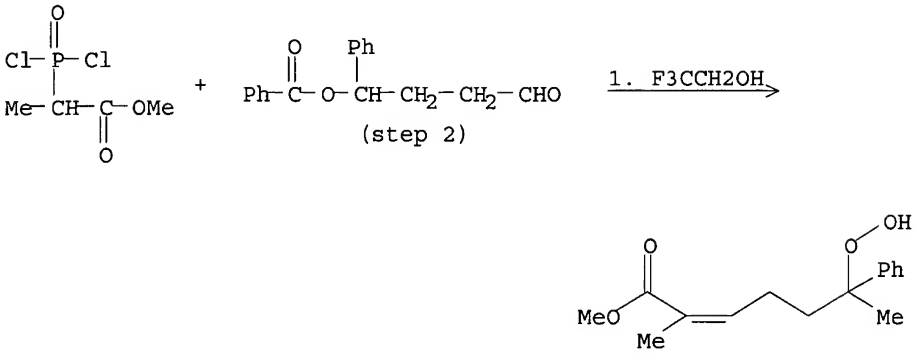


RX(544) OF 707 - 6 STEPS

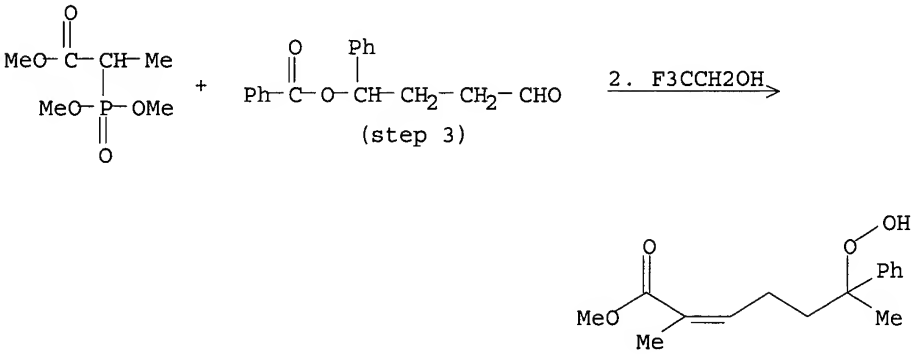




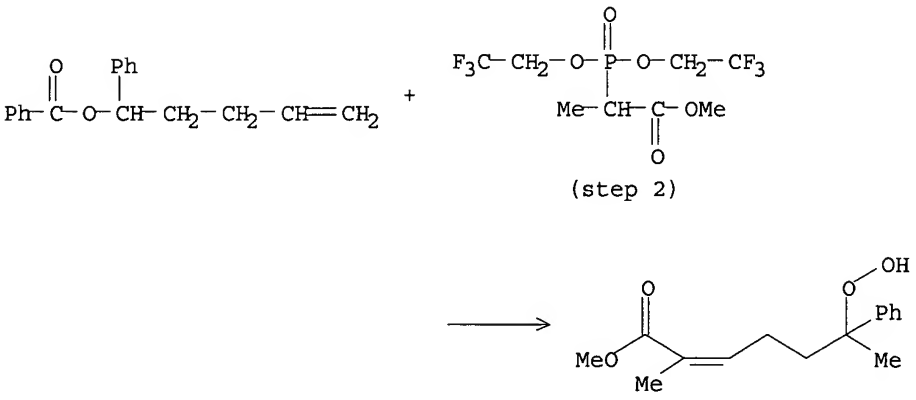
RX(546) OF 707 - 7 STEPS



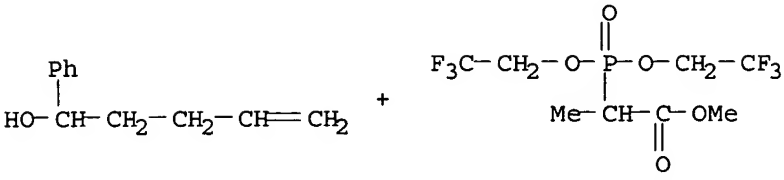
RX(548) OF 707 - 8 STEPS



RX(550) OF 707 - 7 STEPS



RX(552) OF 707 - 8 STEPS



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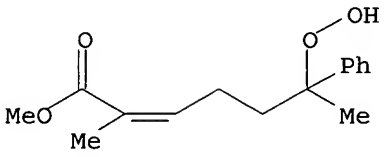
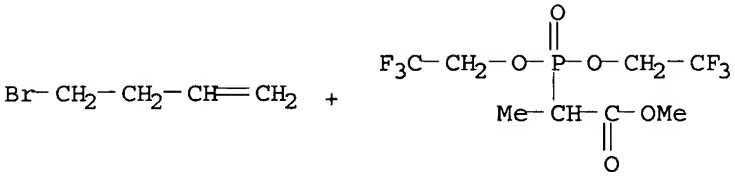


RX(604) OF 707 - 9 STEPS



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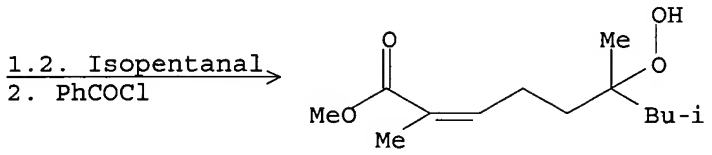
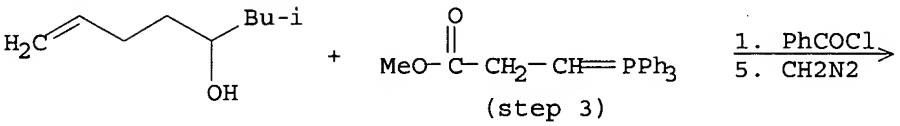
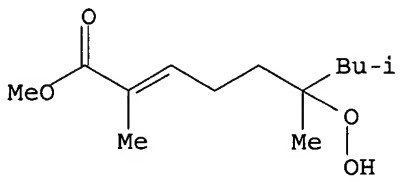


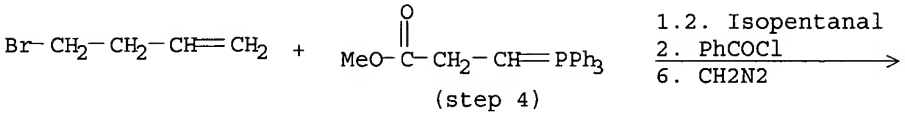
RX(606) OF 707 - 9 STEPS

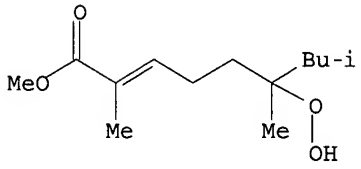


(step 3)

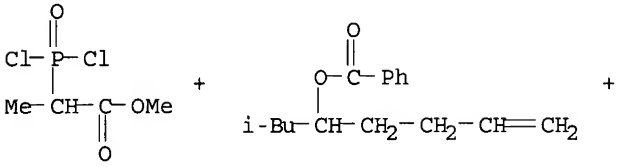


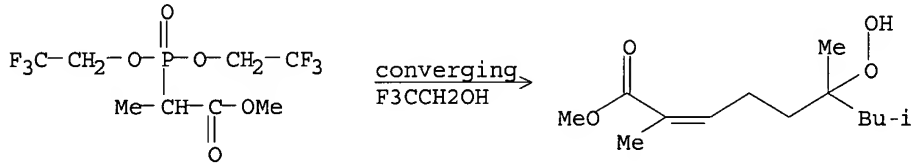
RX(613) OF 707 - 10 STEPS



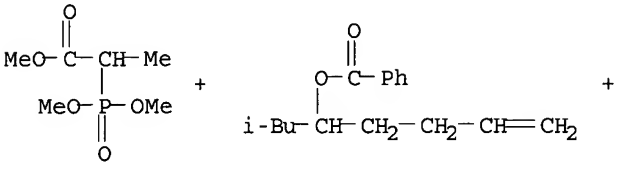


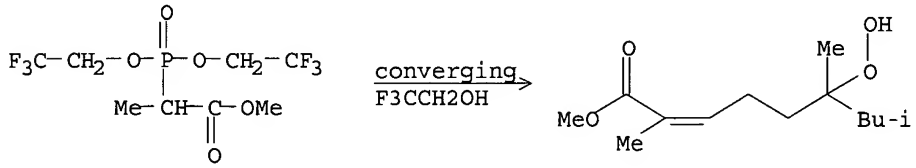
RX(621) OF 707 - 8 STEPS



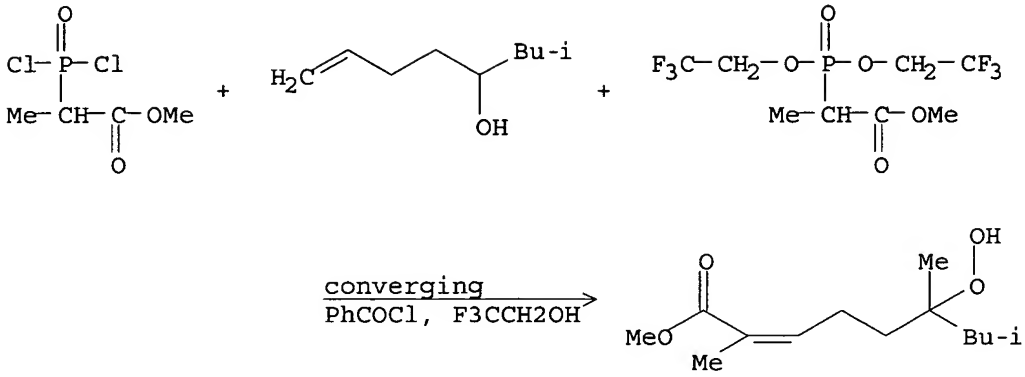


RX(623) OF 707 - 9 STEPS

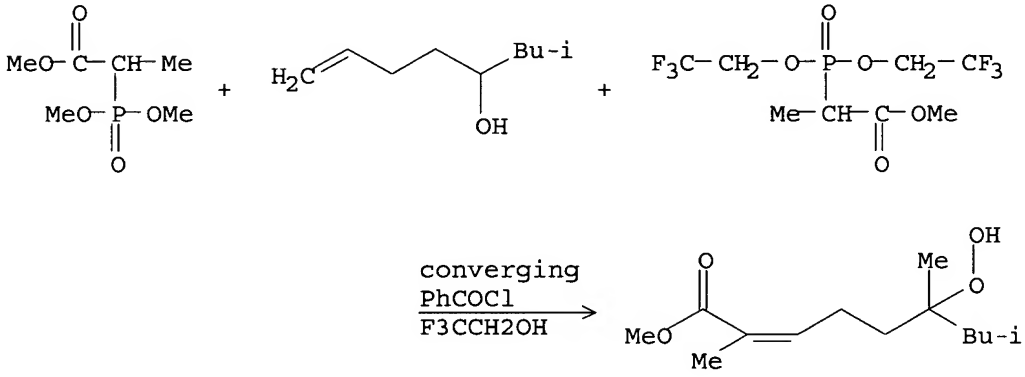




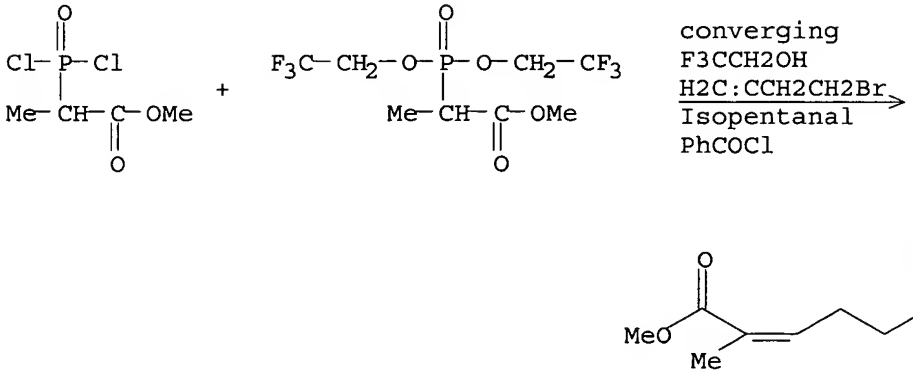
RX(627) OF 707 - 9 STEPS



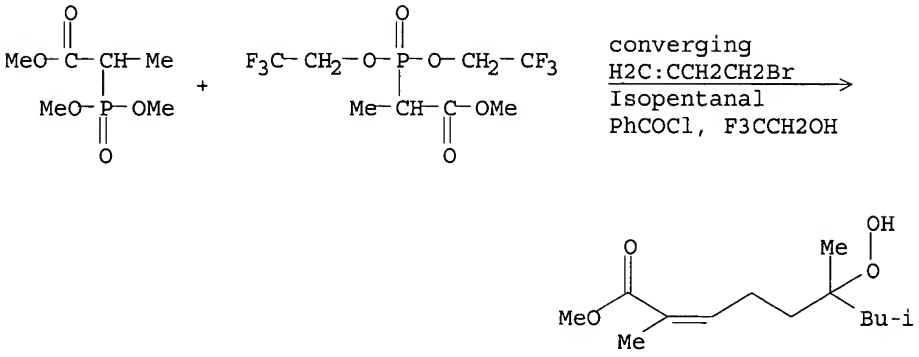
RX(629) OF 707 - 10 STEPS



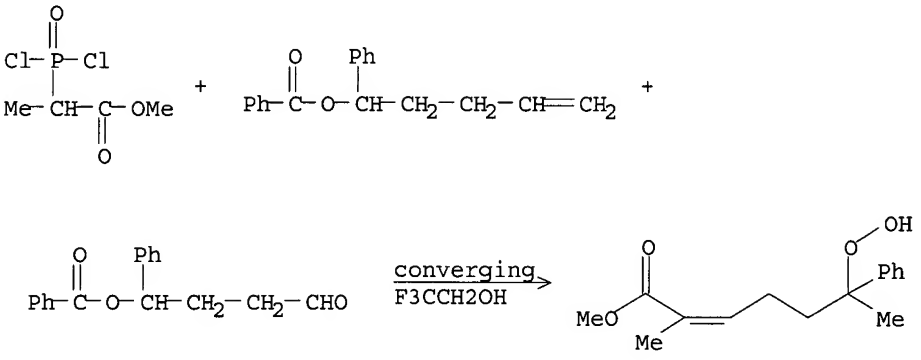
RX(633) OF 707 - 10 STEPS



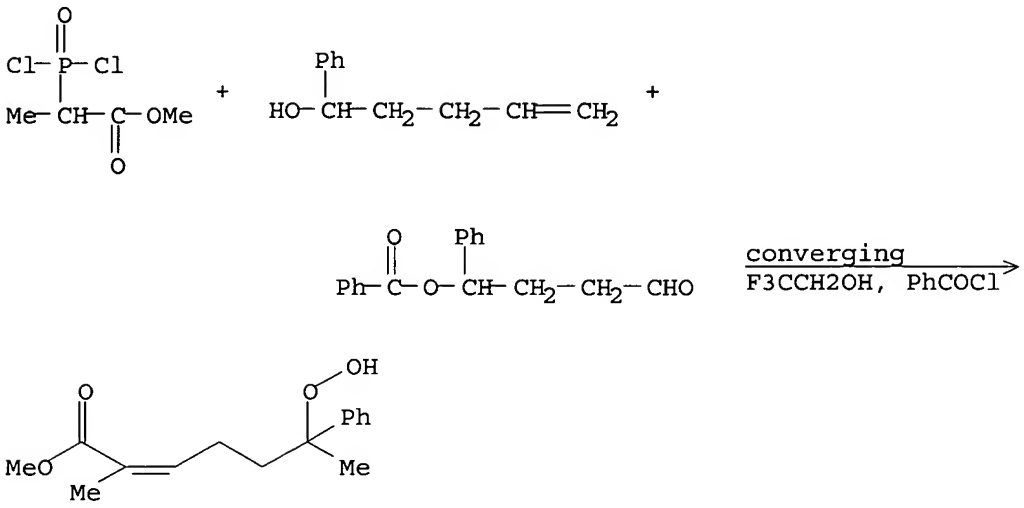
RX(635) OF 707 - 11 STEPS



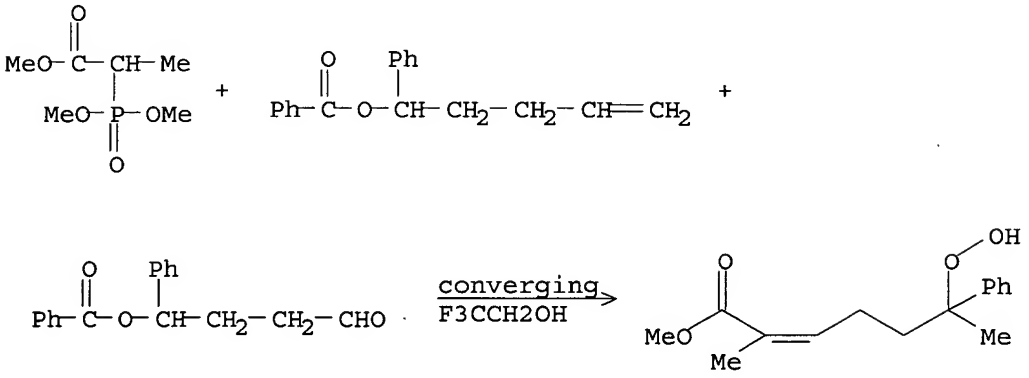
RX(658) OF 707 - 8 STEPS



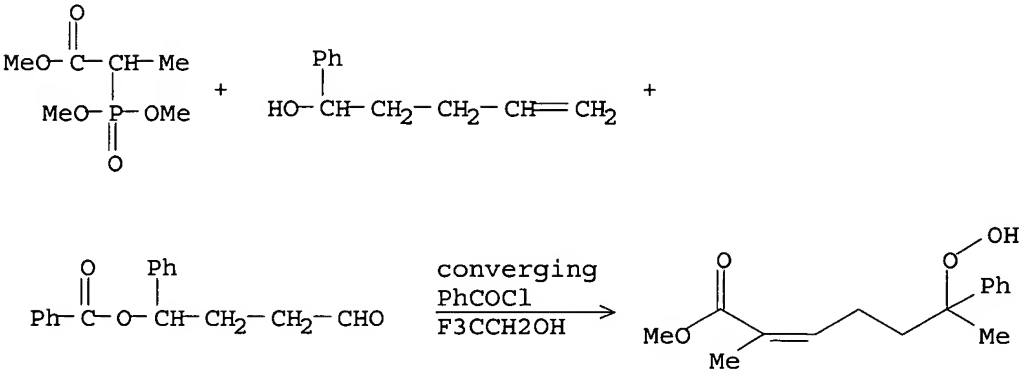
RX(660) OF 707 - 9 STEPS



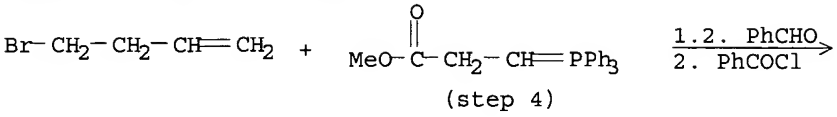
RX(670) OF 707 - 9 STEPS

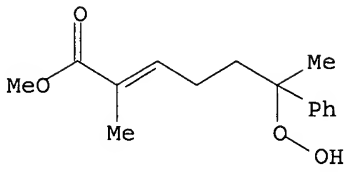


RX(672) OF 707 - 10 STEPS

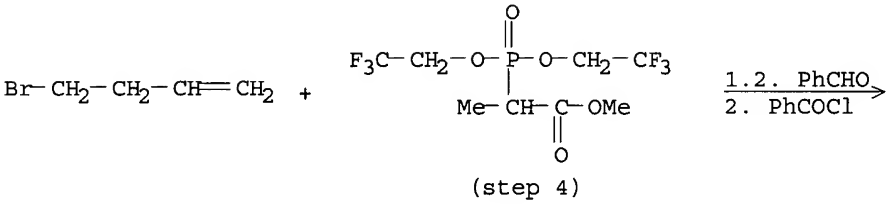


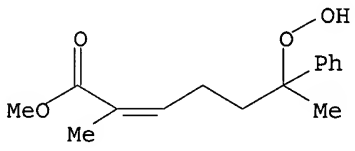
RX(677) OF 707 - 9 STEPS



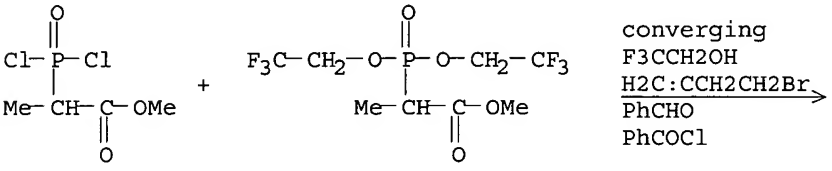


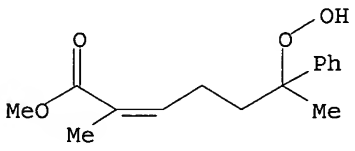
RX(679) OF 707 - 9 STEPS



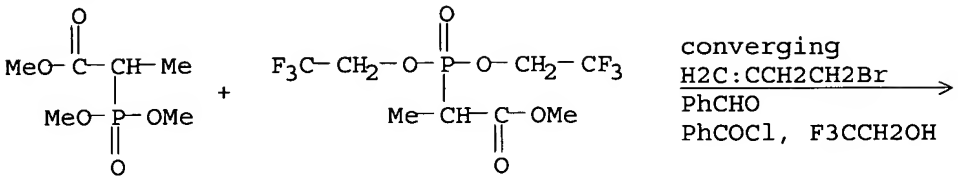


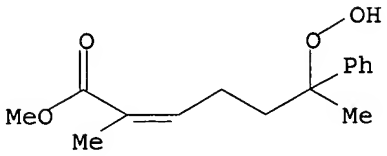
RX(701) OF 707 - 10 STEPS



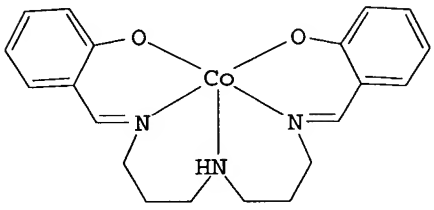


RX(703) OF 707 - 11 STEPS





L34 ANSWER 25 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 105:97096 CASREACT
TITLE: Oxygenation of tert-butylphenols with an unsaturated side chain
AUTHOR(S): Nishinaga, Akira; Iwasaki, Hitoshi; Shimizu, Tadashi; Toyoda, Yasushi; Matsuura, Teru
CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Journal of Organic Chemistry (1986), 51(12), 2257-66
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

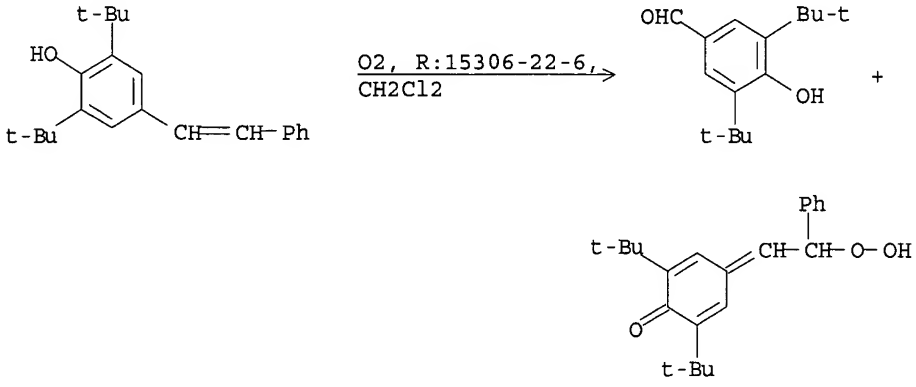


I

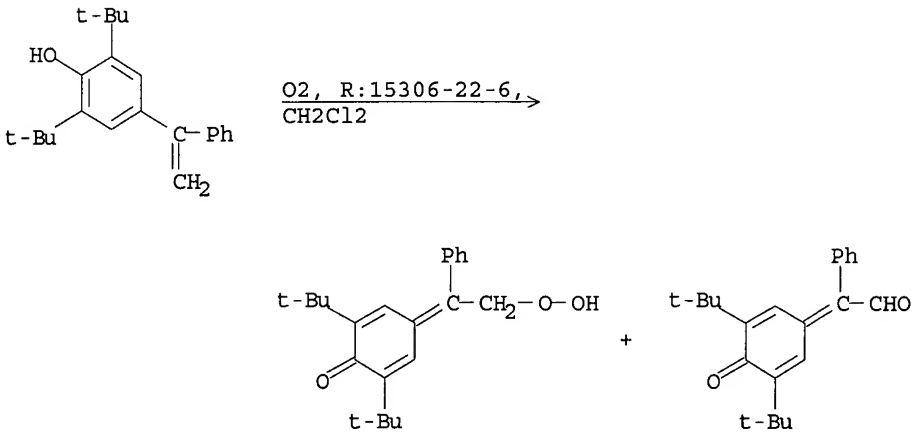
AB Base and Co(Salpr)(I)-promoted oxygenation of the title compds. was studied to obtain details concerning controlling factors in regioselective O2 incorporation into phenols. In the oxygenation of 4-alkenyl-2,6-di-tert-butyl-(II) and 2-alkenyl-4,6-di-tert-butylphenols (III), the reactivity of the substrates and regioselectivity in the O2 incorporation is interpreted in terms of electronic and steric effects of the alkenyl group as well as association effect of the countercation K+ on the transition-state involving a charge-transfer from the substrate anion to O2. With 4-alkynyl-2,6-di-tert-butylphenols (IV), O2 was incorporated exclusively into the ortho position only when the phenolate anion was associated with K+. On the contrary, in the oxygenation of II and III with

I, O2 was incorporated exclusively into the alkenyl side chain, regardless of the nature of the substituent; with IV O2 incorporation was distributed to both the ortho and the alkynyl side chain. The substituent-dependent regioselectivity in the oxygenation of phenols with I is because the reactive phenolate-Co(III) species undergo homolysis to form phenoxy radical-Co(II) species reversibly, whose oxygenations complete with each other. When the oxygenation of the anionic species predominates, O2 is incorporated into the ortho position; with the radical species the para and side chain oxidns. predominate.

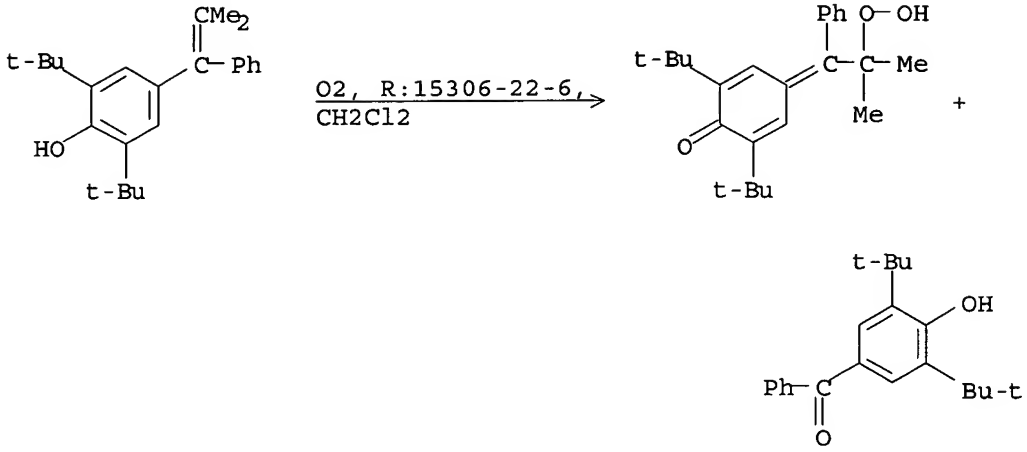
RX(30) OF 164



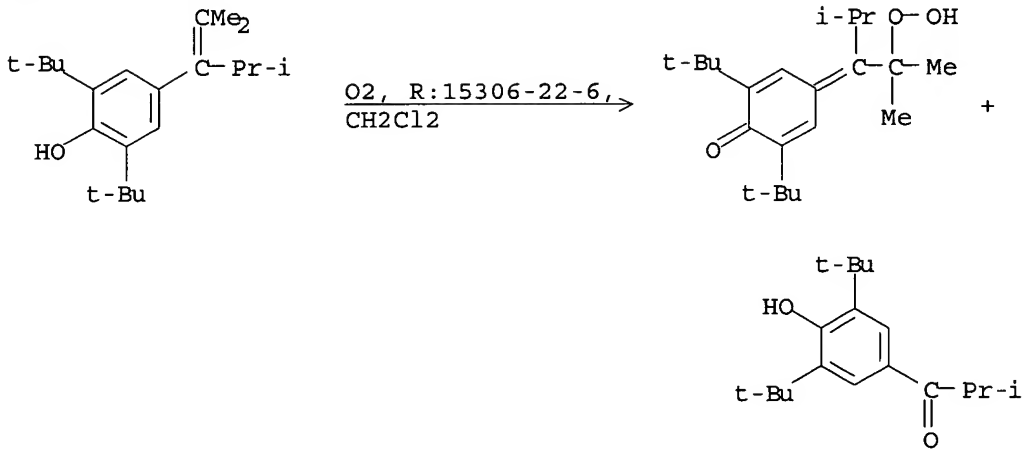
RX(31) OF 164



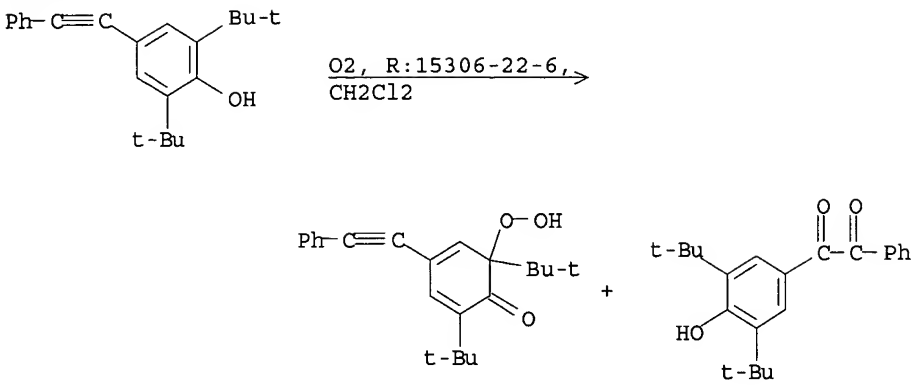
RX(32) OF 164



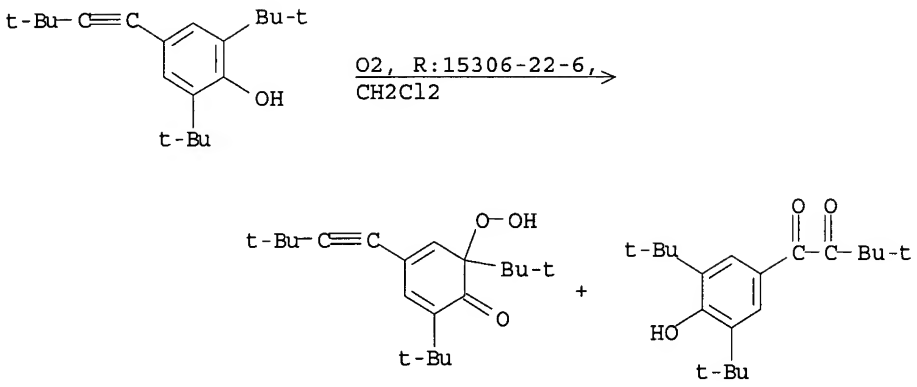
RX(33) OF 164



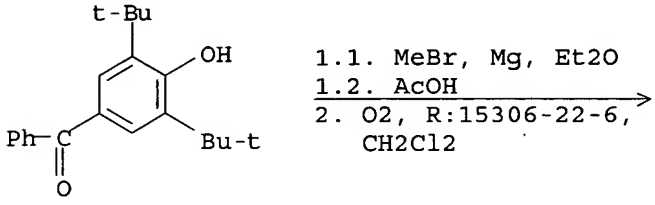
RX(64) OF 164

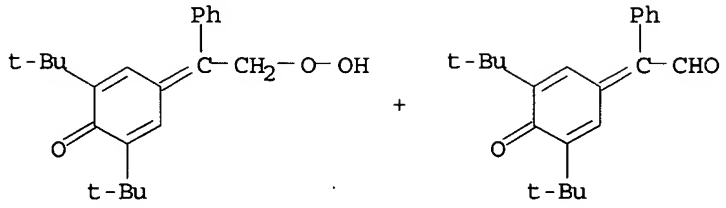


RX(66) OF 164



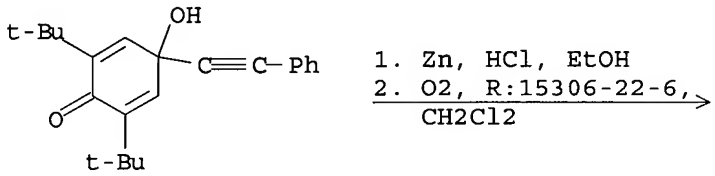
RX(74) OF 164 - 2 STEPS

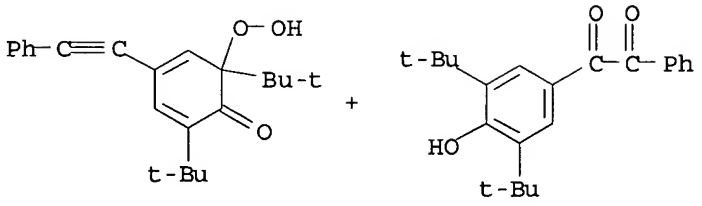




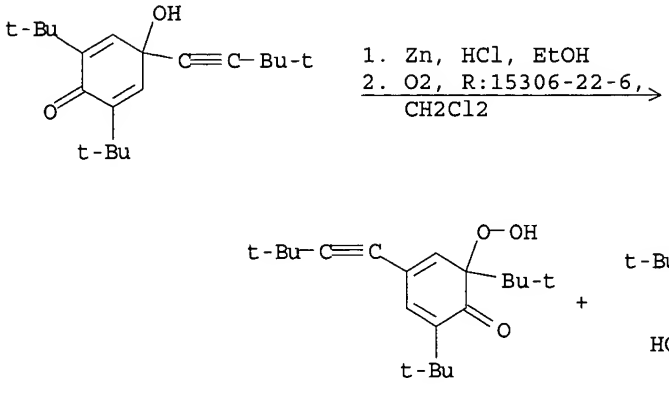
NOTE: 1) alkyl bromide assumed

RX(116) OF 164 - 2 STEPS

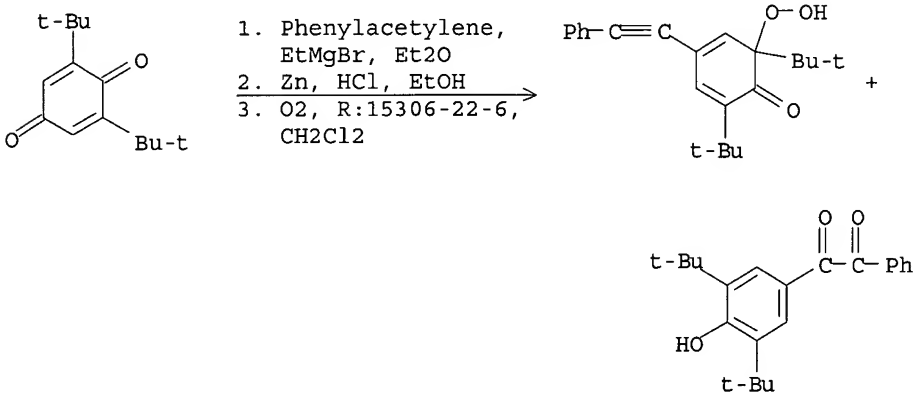




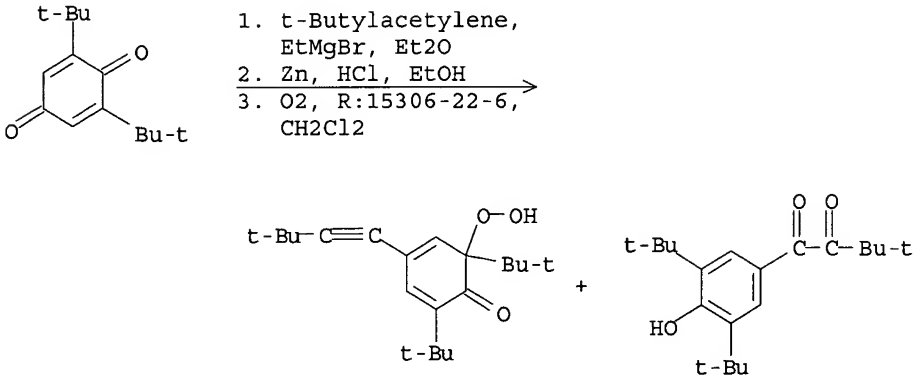
RX(120) OF 164 - 2 STEPS



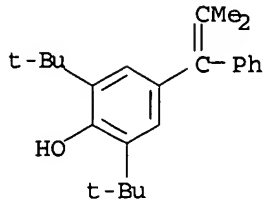
RX(154) OF 164 - 3 STEPS



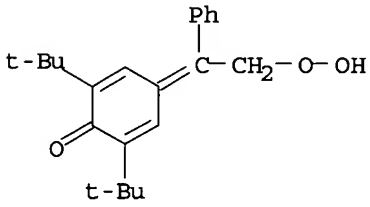
RX(158) OF 164 - 3 STEPS



RX(161) OF 164 - 3 STEPS



1. O2, R:15306-22-6, CH2Cl2
2.1. MeBr, Mg, Et2O
2.2. AcOH
3. O2, R:15306-22-6, CH2Cl2



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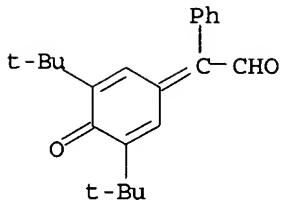
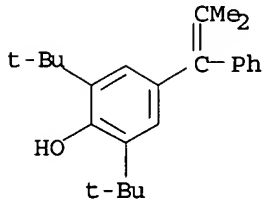
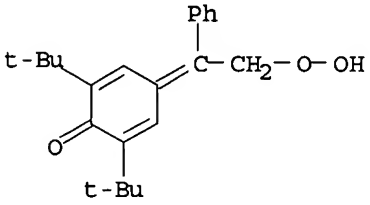


NOTE: 2) alkyl bromide assumed

RX(162) OF 164 - 3 STEPS



1. O2, t-BuOK, DMF
2.1. MeBr, Mg, Et2O
2.2. AcOH
3. O2, R:15306-22-6, CH2Cl2



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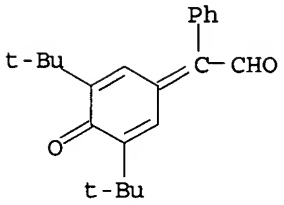
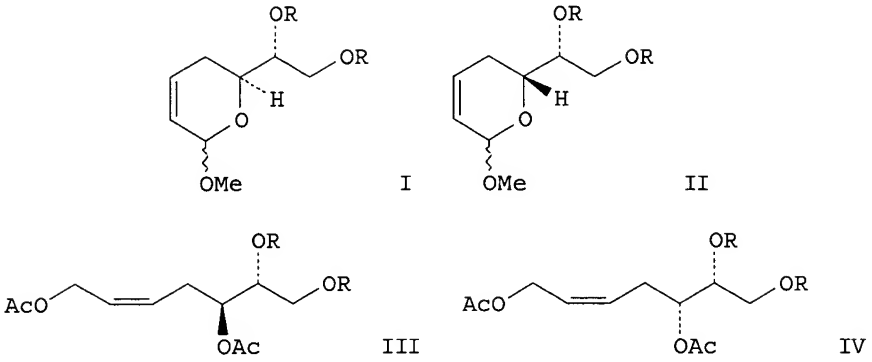


NOTE: 2) alkyl bromide assumed

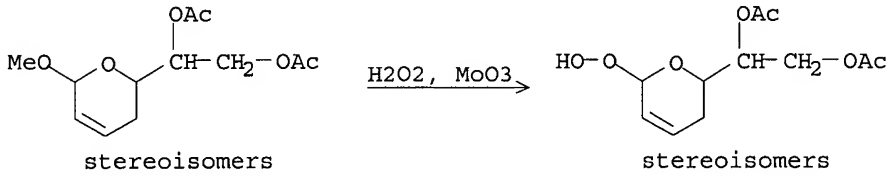
L34 ANSWER 26 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 106:102630 CASREACT
TITLE: Novel reductive opening of 5,6-dihydro-2H-pyran ring
AUTHOR(S): Jurczak, Janusz; Bauer, Tomasz; Ankner, Kjell
CORPORATE SOURCE: Inst. Org. Chem., Pol. Acad. Sin., Warsaw, 01-224, Pol.
SOURCE: Heterocycles (1986), 24(6), 1531-4
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal
LANGUAGE: English
GI

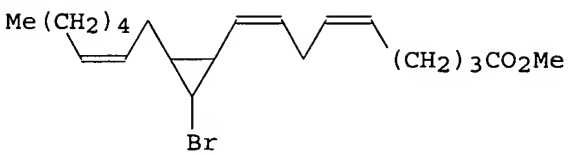


AB Methoxydihydropyrans I (R = Ac, PhCH2) and II (R = Ac, PhCH2) on oxidation with H2O2 in the presence of MoO3, followed by reduction of the resulting peroxides with NaBH4 and then acetylation with Ac2O gave enantiomerically pure open-chain compds. III and IV (same R), resp. III and IV can serve as chiral building blocks in the synthesis of natural products.

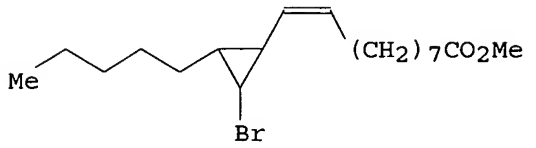
RX(1) OF 11



L34 ANSWER 27 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 103:122958 CASREACT
TITLE: General synthesis of polyunsaturated fatty acid hydroperoxides involving a novel vinylcyclopropyl bromide ring opening
AUTHOR(S): Porter, N. A.; Ziegler, C. B., Jr.; Khouri, F. F.; Roberts, D. H.
CORPORATE SOURCE: P. M. Gross Chem. Lab., Duke Univ., Durham, NC, 27706, USA
SOURCE: Journal of Organic Chemistry (1985), 50(13), 2252-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



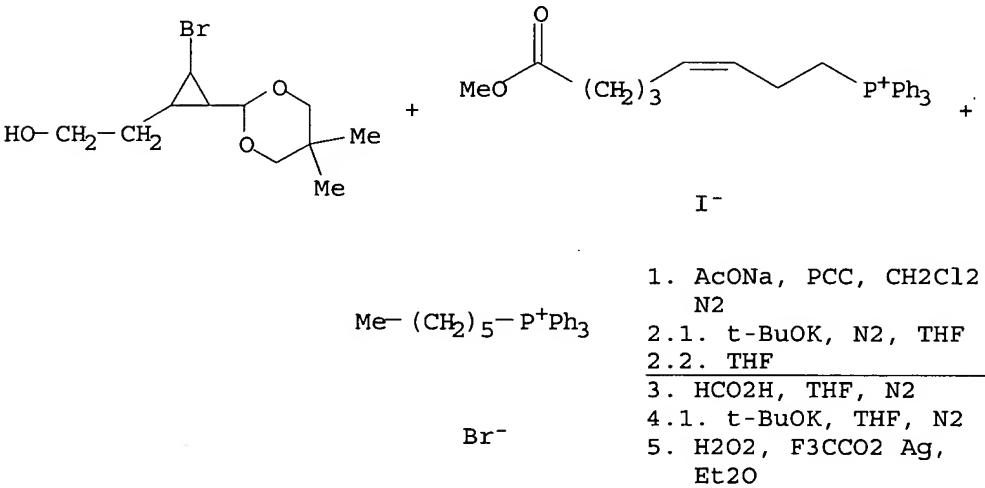
I



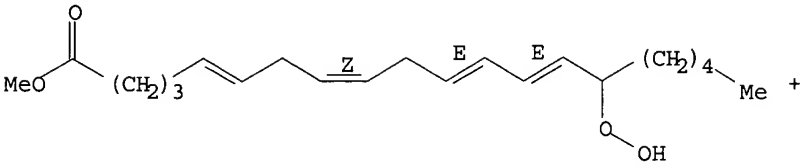
II

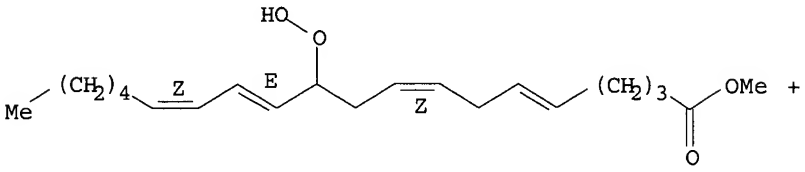
AB A variety of 18- and 20-carbon polyunsatd. fatty acid hydroperoxides were synthesized via an orbital symmetry controlled ring opening of vinylcyclopropyl bromides. Six 20-carbon vinylcyclopropyl bromides, e.g. I were synthesized by a route starting from 2-ethoxy-Δ3,5-dihydropyran and an 18-carbon vinylcyclopropyl bromide II by a route starting from propargyl alc. All six vinylcyclopropyl bromides underwent facile Ag+-assisted ring opening in the presence of excess H2O2 to form the target fatty acid hydroperoxide isomers in good yields. In most cases the products were produced with stereochem. control. The product hydroperoxides formed in this ring-opening reaction are consistent with a mechanism involving the formation of a pentadienyl cation intermediate. A minor product found in the reaction of II provides evidence that homoallylic participation by alkenyl substituents can change the course of the electrocyclic ring opening.

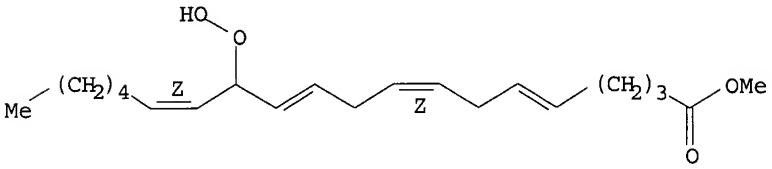
RX(102) OF 133 - 5 STEPS



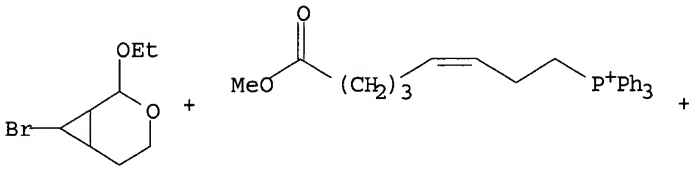
RX(102) OF 133 - 5 STEPS

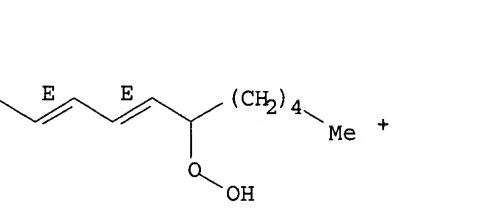




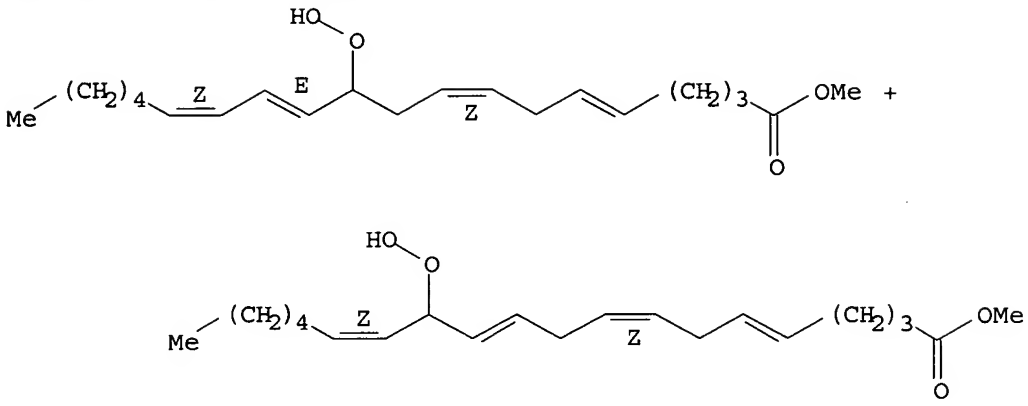


RX(103) OF 133 - 6 STEPS

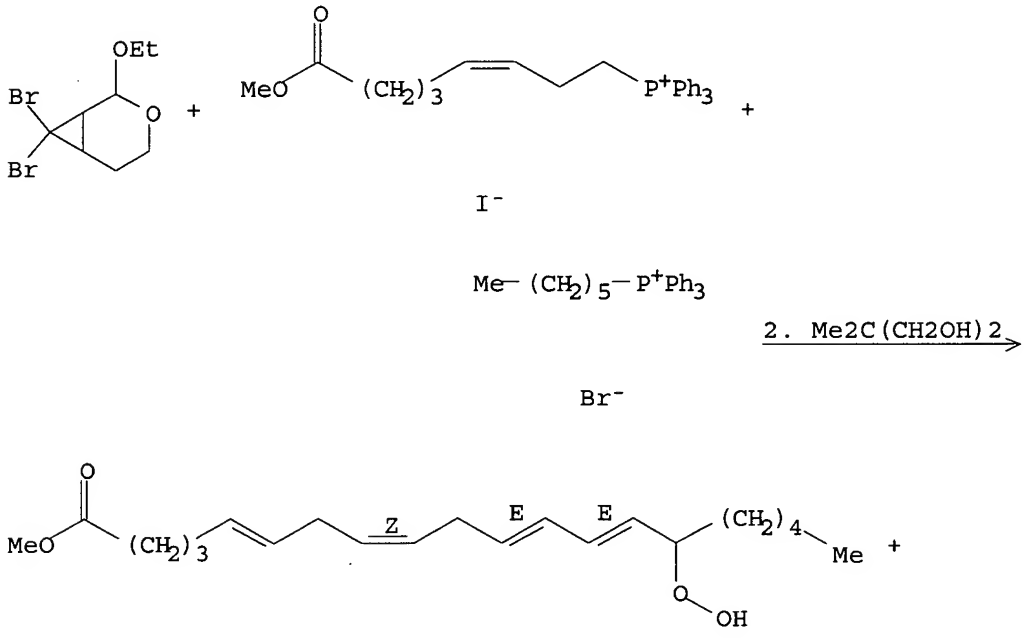




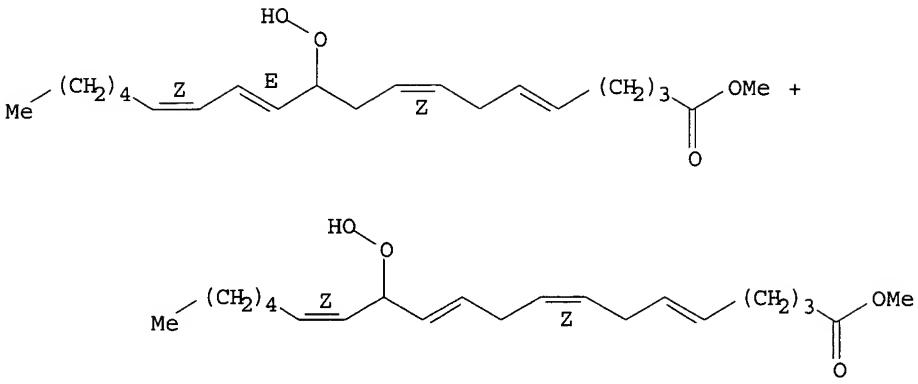
RX(103) OF 133 - 6 STEPS



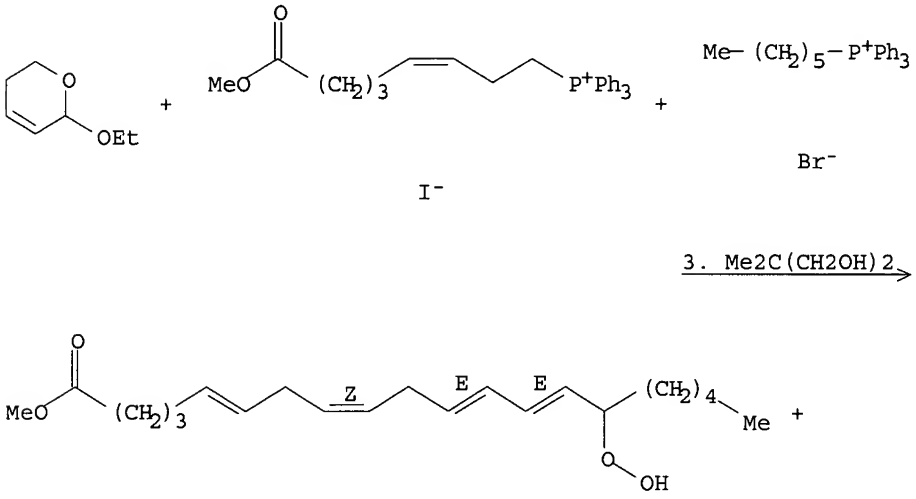
RX(104) OF 133 - 7 STEPS



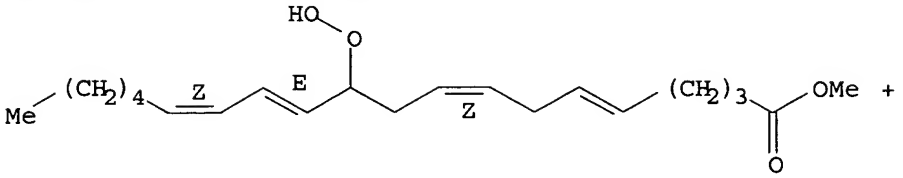
RX(104) OF 133 - 7 STEPS

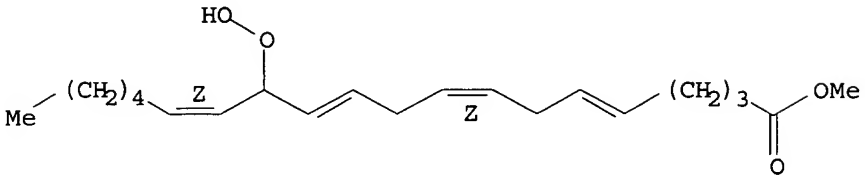


RX(105) OF 133 - 8 STEPS



RX(105) OF 133 - 8 STEPS

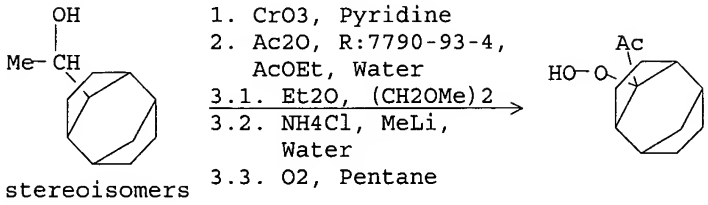




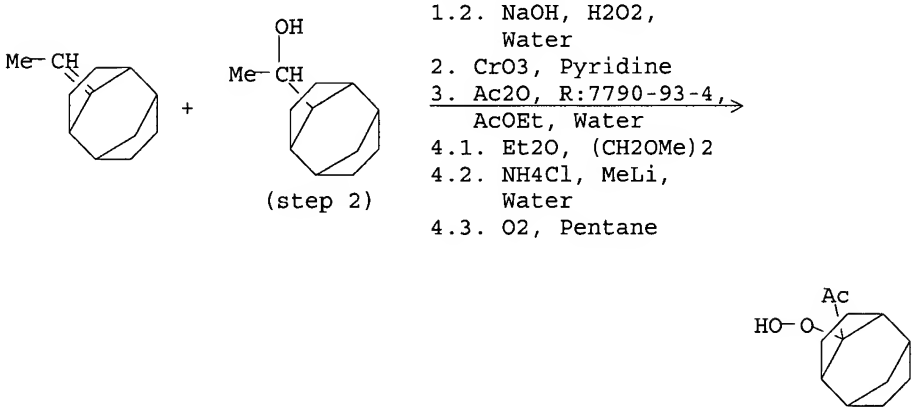
L34 ANSWER 28 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 102:203393 CASREACT
TITLE: Enhanced endo-exo selectivity in the stereochemistry of ketonization of enols. Part 201
AUTHOR(S): Zimmerman, Howard E.; Linder, Linus W.
CORPORATE SOURCE: Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Journal of Organic Chemistry (1985), 50(10), 1637-46
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The enols of 9-acetyl-anti-tricyclo[4.2.1.12,5]decane (I) and 9-benzoyl-anti-tricyclo[4.2.1.12,5]decane (II) were generated by reaction of the bromo ketone with mercaptans or with dilute HI in acetone, or by conversion of the enol acetates to the enolates followed by protonation. The enol of I was also generated by photolysis of the enoloxy dimer (III). The enols were stable with half-lives ranging from a half hour to more than 24 h, depending on conditions. The presence of the enols was monitored by reaction with O2. III was formed when the α-bromo(acetyl)tricyclic was irradiated in Me2CHOH containing NaOAc; III had two enoloxy radicals bonded from the C(α) atom of one to the enoloxy oxygen of the second. Base-catalyzed equilibration of the ketones led to the endo and the exo isomers with a product ratio less than 1 to 1000. Enol ketonization occurs with exo attack, giving the endo isomers, (the endo isomers are preferred by at least 3300 to 1). The very large kinetic preference for the less stable endo ketone isomer results from steric hindrance by the C(3) and C(5) axial CH2 groups blocking the endo approach of proton donors. A MM2 treatment of the stereochem. of ketonization revealed the expected preference for exo protonation of both the tricyclic enol (observed in the present study) and also unsubstituted exocyclic 6-ring enols. For the 2-phenyl-1-acetyl system, the axial Ph conformer of starting material was preferred. However, for the protonation transition state, the equatorial Ph conformer with exo protonation was lowest in energy. Next was the axial Ph conformer with axial protonation. Third was the axial Ph conformer with exo protonation, and least stable was the equatorial Ph conformer with endo protonation.

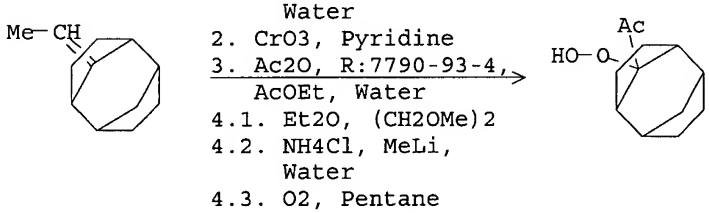
RX(103) OF 447 - 3 STEPS



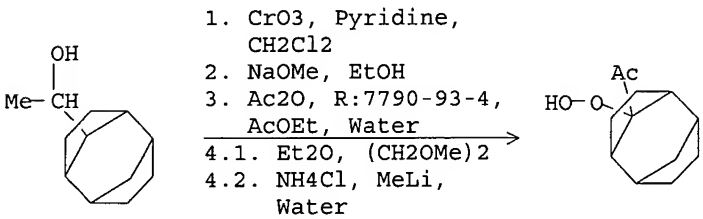
RX(104) OF 447 - 4 STEPS



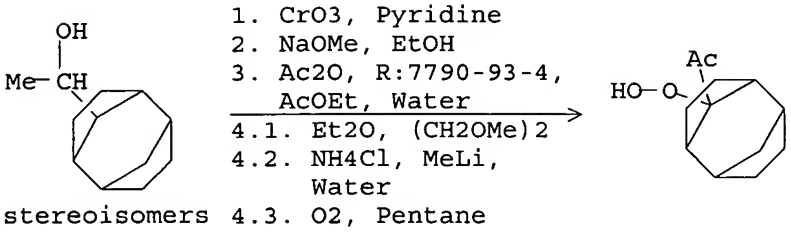
RX(105) OF 447 - 4 STEPS



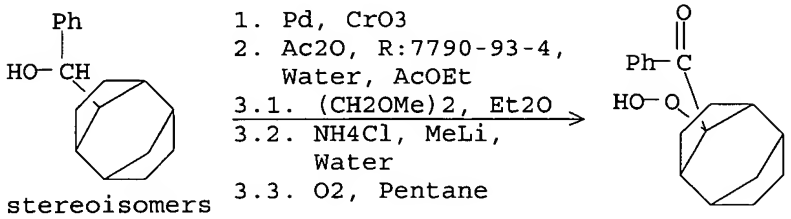
RX(106) OF 447 - 4 STEPS



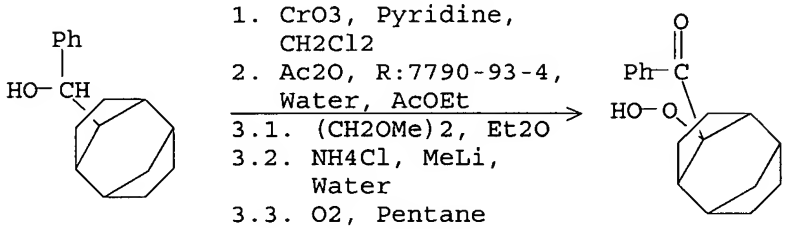
RX(112) OF 447 - 4 STEPS



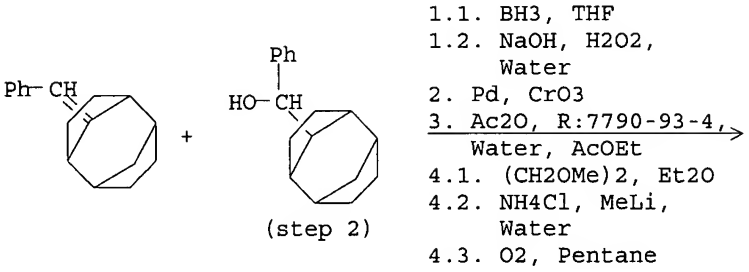
RX(169) OF 447 - 3 STEPS

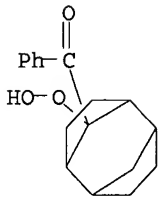


RX(170) OF 447 - 3 STEPS



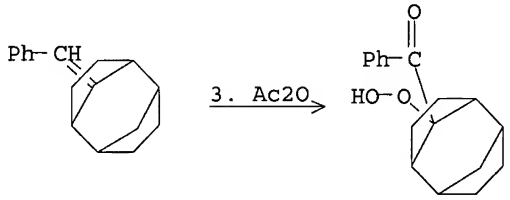
RX(173) OF 447 - 4 STEPS





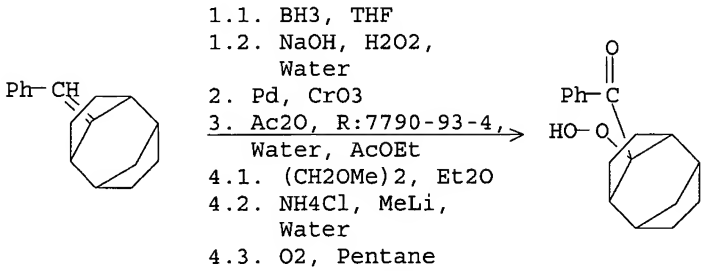
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(174) OF 447 - 4 STEPS



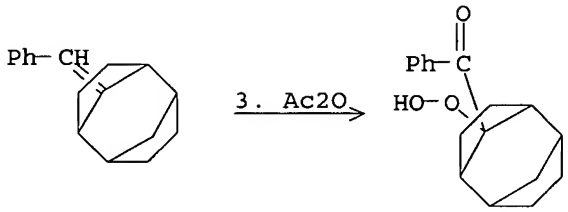
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(175) OF 447 - 4 STEPS



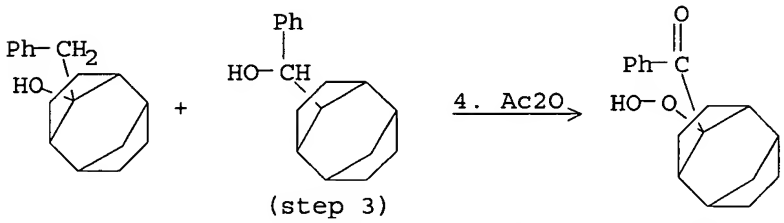
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(176) OF 447 - 4 STEPS



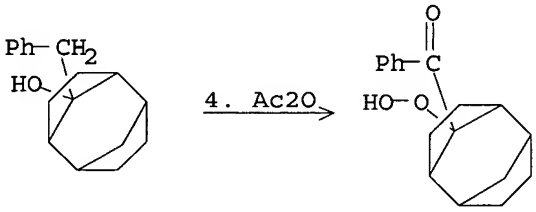
NOTE: 1) exo/endo ratio dependent on reflux of oxidative reference

RX(313) OF 447 - 5 STEPS



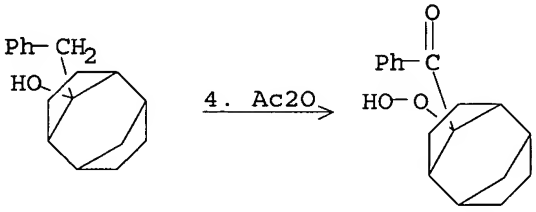
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(314) OF 447 - 5 STEPS



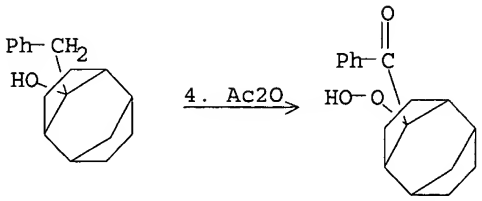
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(315) OF 447 - 5 STEPS



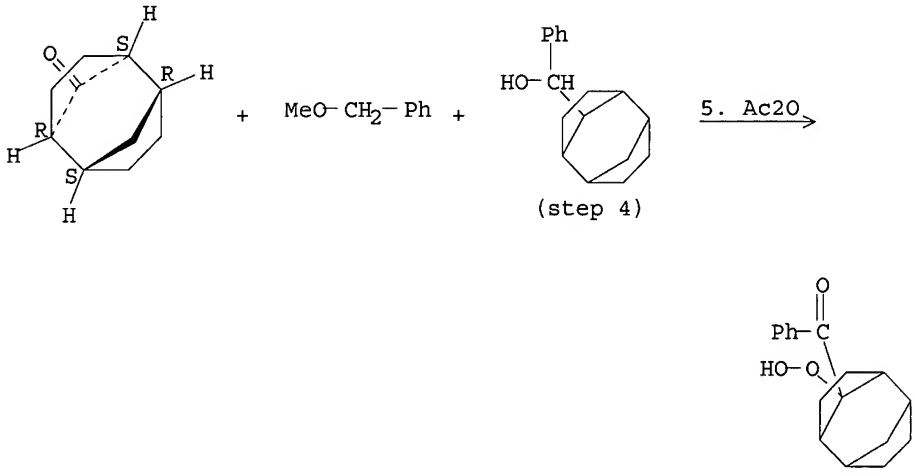
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(316) OF 447 - 5 STEPS



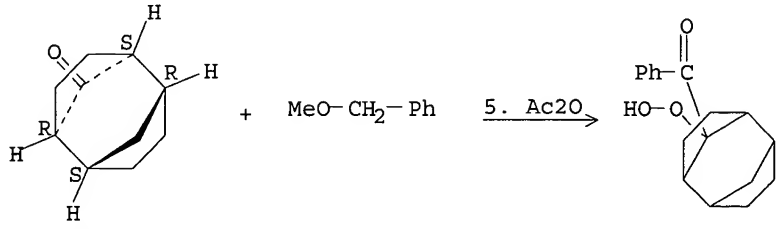
NOTE: 2) exo/endo ratio dependent on reflux of oxidative reference

RX(329) OF 447 - 6 STEPS



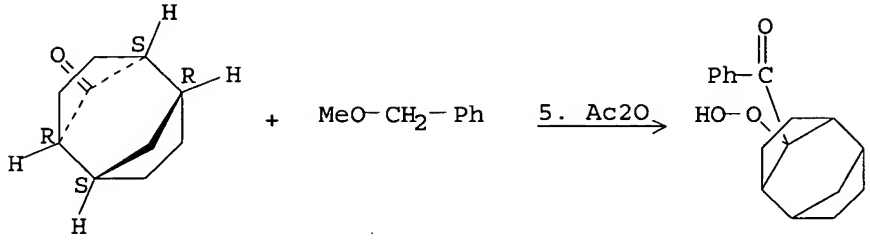
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(330) OF 447 - 6 STEPS



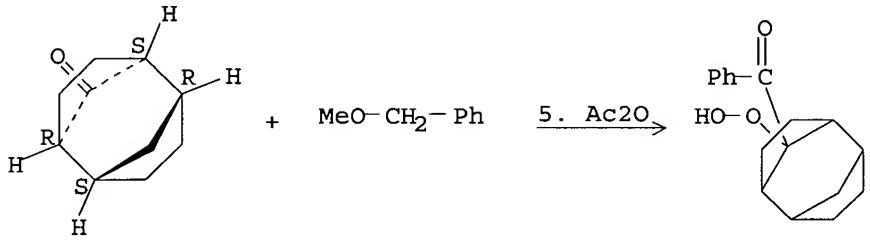
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(331) OF 447 - 6 STEPS



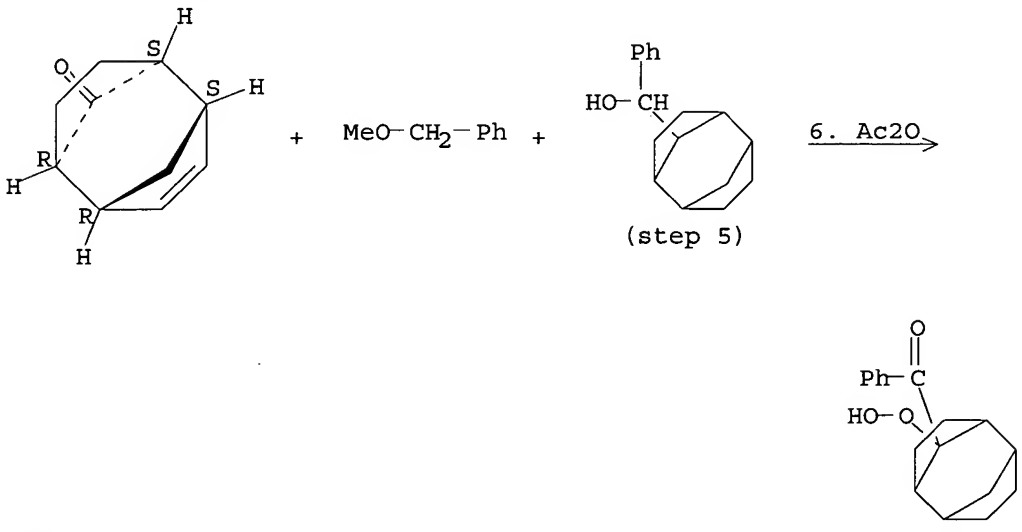
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(332) OF 447 - 6 STEPS



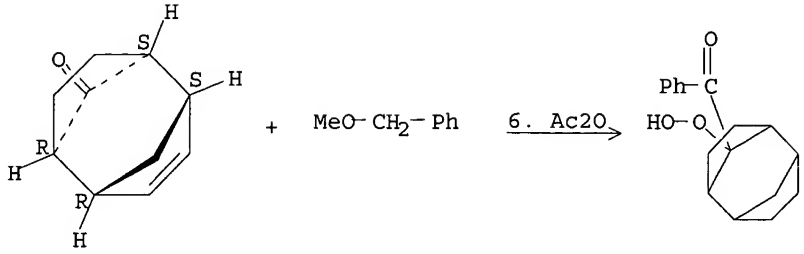
NOTE: 3) exo/endo ratio dependent on reflux of oxidative reference

RX(345) OF 447 - 7 STEPS



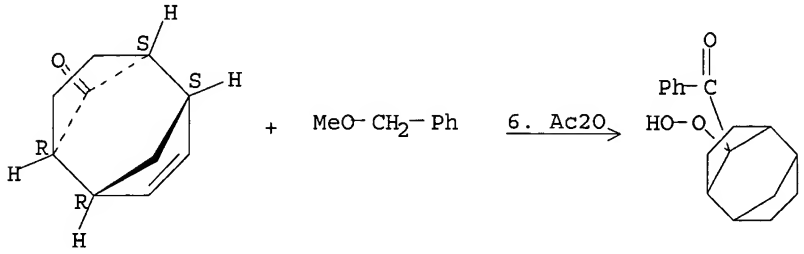
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(346) OF 447 - 7 STEPS



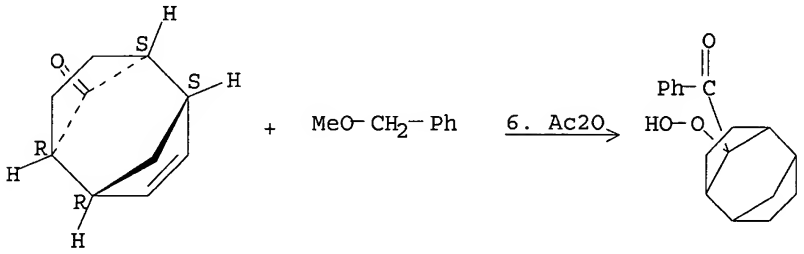
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(347) OF 447 - 7 STEPS



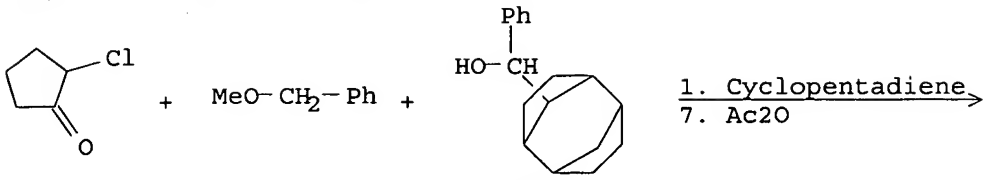
NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(348) OF 447 - 7 STEPS

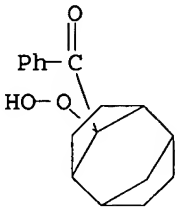


NOTE: 4) exo/endo ratio dependent on reflux of oxidative reference

RX(361) OF 447 - 8 STEPS

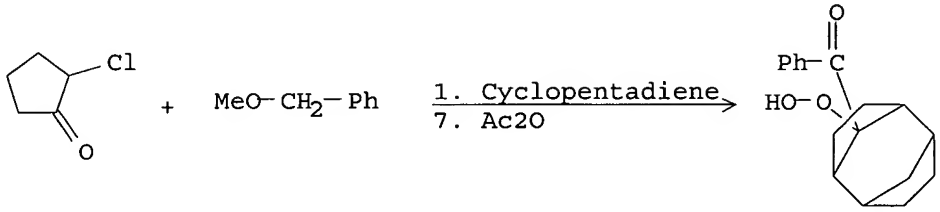


(step 6)



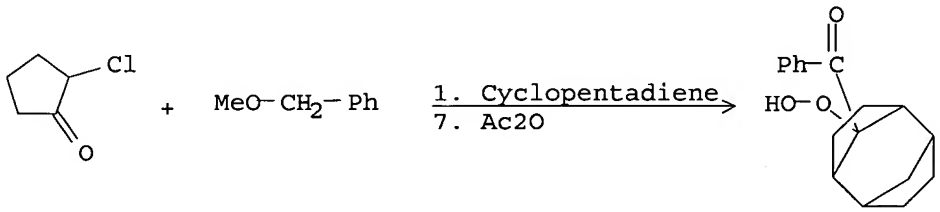
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(362) OF 447 - 8 STEPS



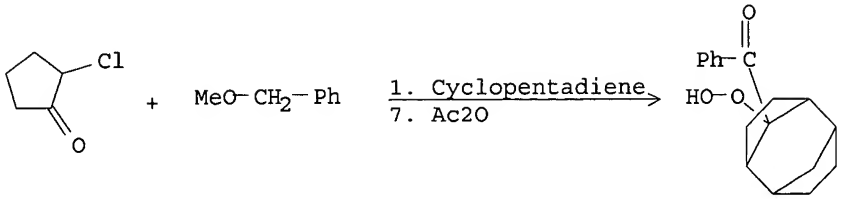
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(363) OF 447 - 8 STEPS



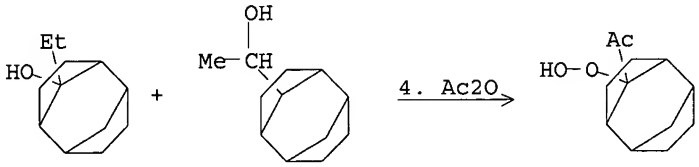
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(364) OF 447 - 8 STEPS



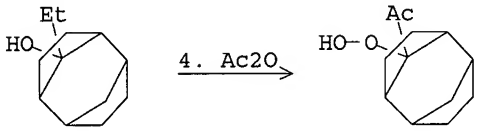
NOTE: 5) exo/endo ratio dependent on reflux of oxidative reference

RX(381) OF 447 - 5 STEPS

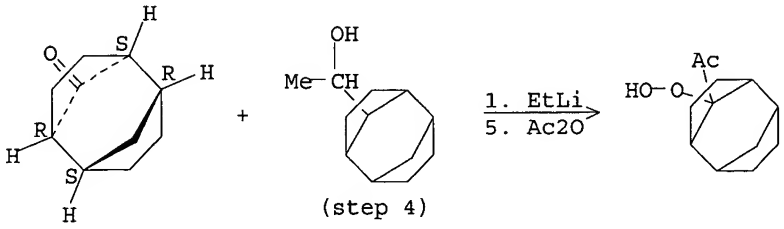


(step 3)

RX(382) OF 447 - 5 STEPS

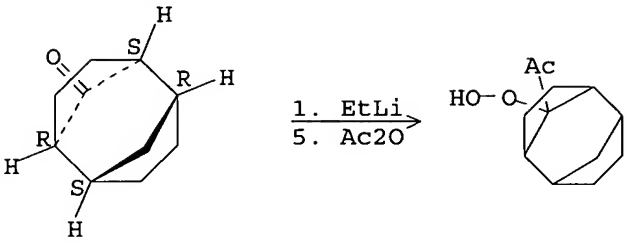


RX(387) OF 447 - 6 STEPS

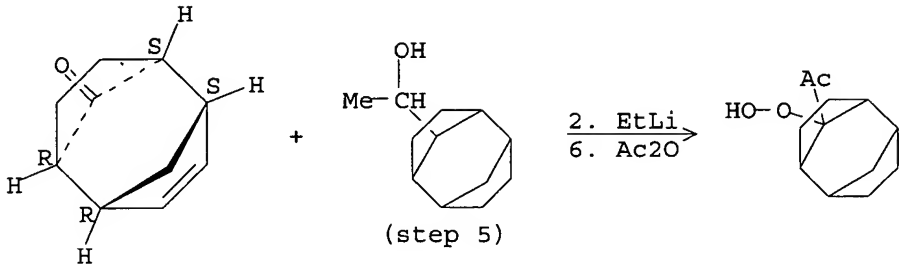


(step 4)

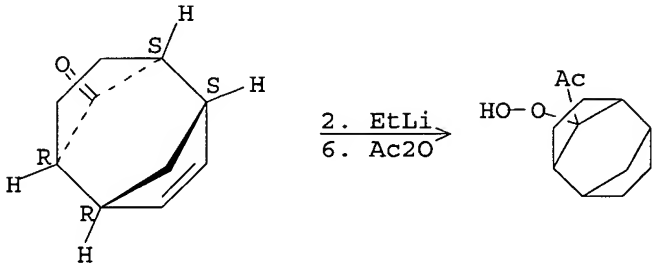
RX(388) OF 447 - 6 STEPS



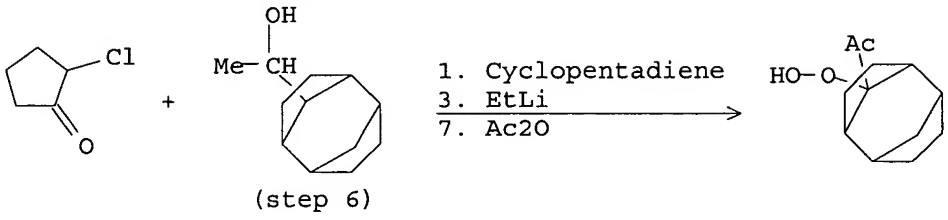
RX(393) OF 447 - 7 STEPS



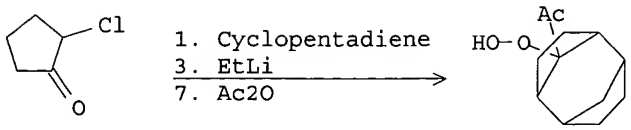
RX(394) OF 447 - 7 STEPS



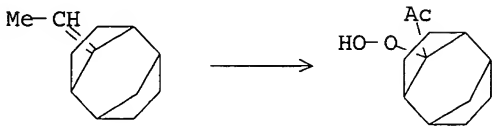
RX(399) OF 447 - 8 STEPS



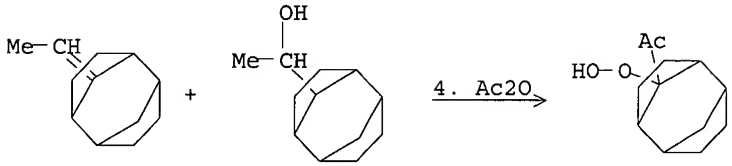
RX(400) OF 447 - 8 STEPS



RX(405) OF 447 - 5 STEPS

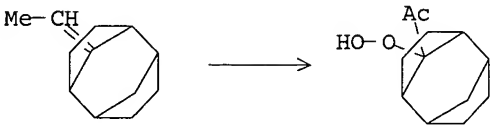


RX(406) OF 447 - 5 STEPS

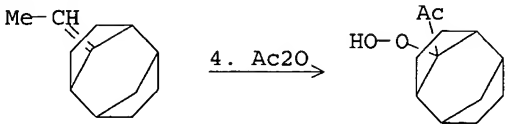


(step 2)

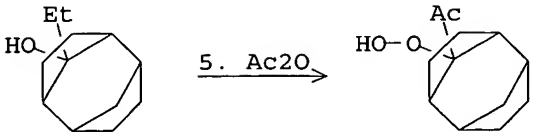
RX(407) OF 447 - 5 STEPS



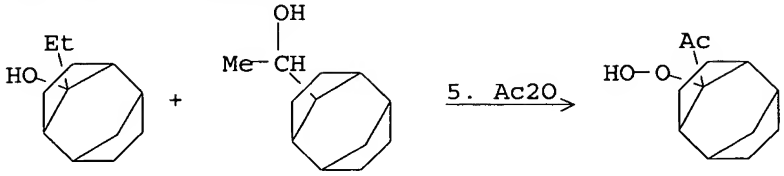
RX(408) OF 447 - 5 STEPS



RX(409) OF 447 - 6 STEPS

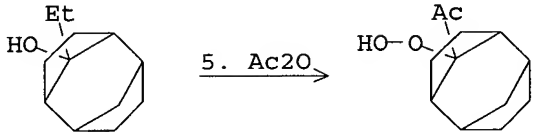


RX(410) OF 447 - 6 STEPS

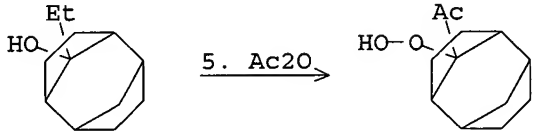


(step 3)

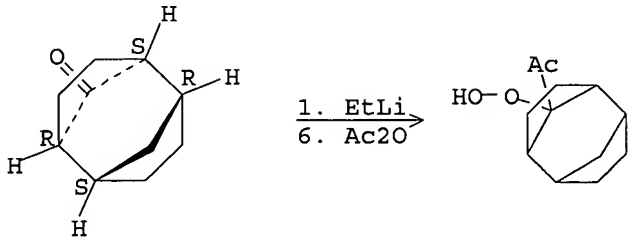
RX(411) OF 447 - 6 STEPS



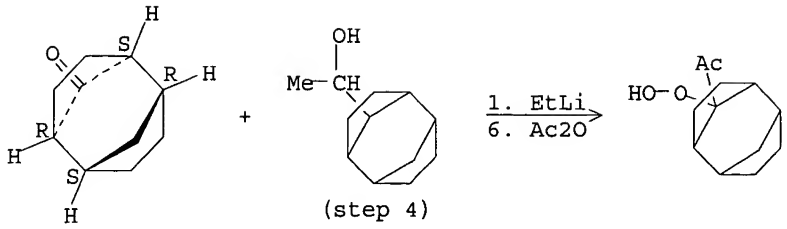
RX(412) OF 447 - 6 STEPS



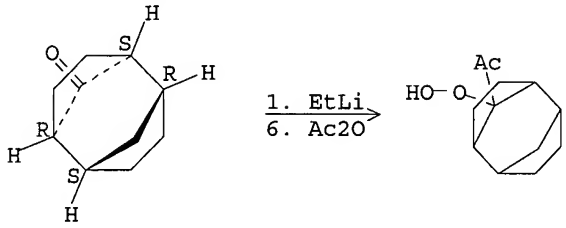
RX(413) OF 447 - 7 STEPS



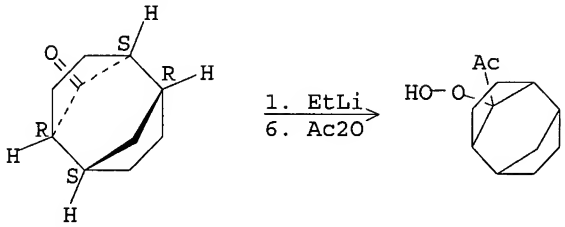
RX(414) OF 447 - 7 STEPS



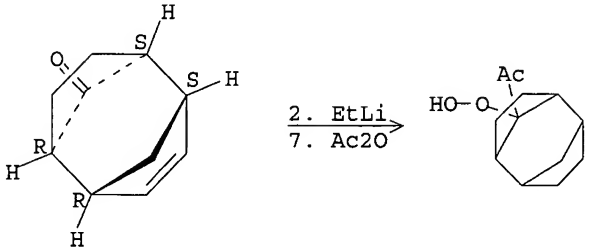
RX(415) OF 447 - 7 STEPS



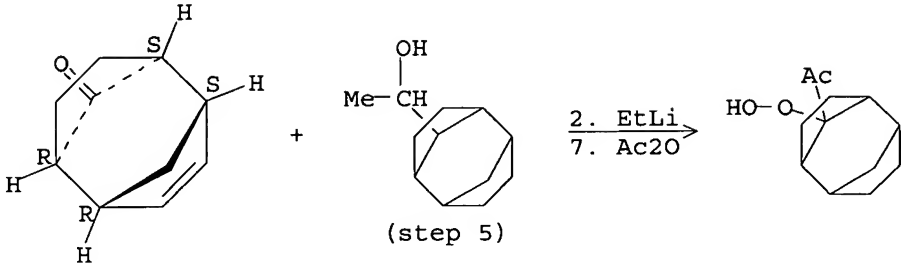
RX(416) OF 447 - 7 STEPS



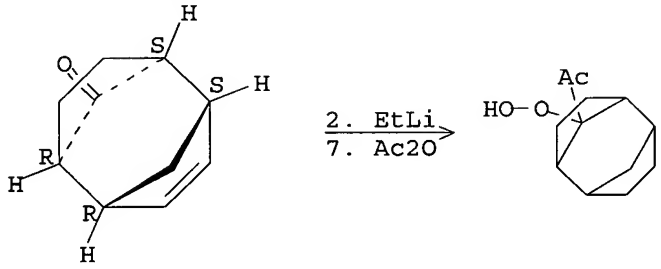
RX(417) OF 447 - 8 STEPS



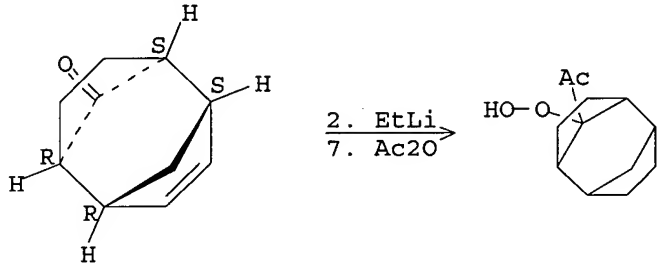
RX(418) OF 447 - 8 STEPS



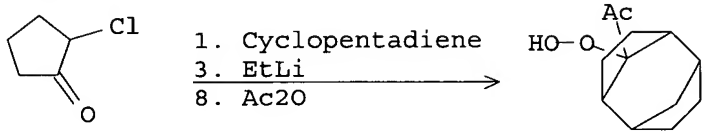
RX(420) OF 447 - 8 STEPS



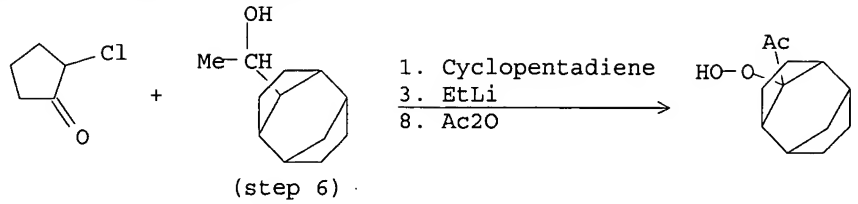
RX(421) OF 447 - 8 STEPS



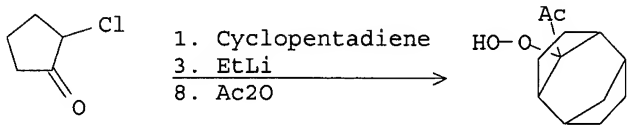
RX(440) OF 447 - 9 STEPS



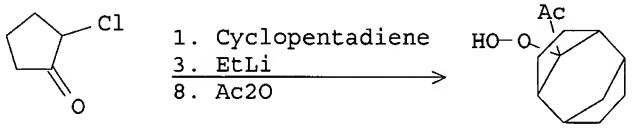
RX(441) OF 447 - 9 STEPS



RX(442) OF 447 - 9 STEPS

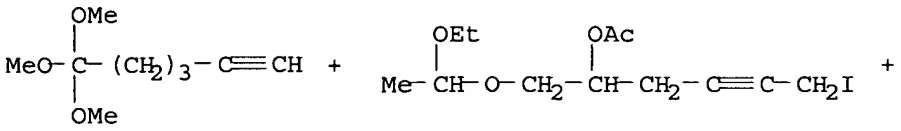


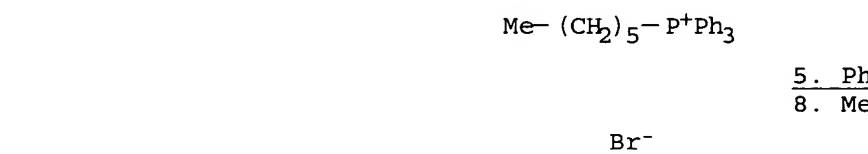
RX(443) OF 447 - 9 STEPS

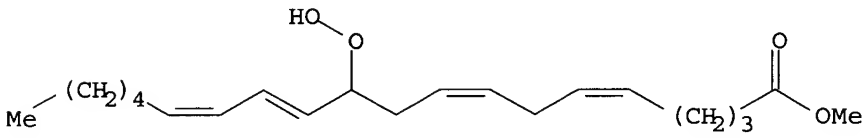


L34 ANSWER 29 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 99:21926 CASREACT
TITLE: The synthesis of 11R- and 11S-HETE [(5Z, 8Z, 12E, 14Z)-11-hydroxyeicosatetraenoic acid] and of 11-R,S-HPETE [(5Z, 8Z, 12E, 14Z)-11-hydroperoxyeicosatetraenoic acid] methyl esters
AUTHOR(S): Just, George; Luthe, Corinne; Viet, Minh Tan Phan
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3A 2K6, Can.
SOURCE: Canadian Journal of Chemistry (1983), 61(4), 712-17
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Me (11R)- and (11S)-hydroxyeicosa-(5Z,8Z,12E,14Z)-tetraenoate (S-I) and the corresponding 11-hydroperoxide were prepared from readily available starting materials. 1H nmr studies of I were undertaken to confirm the structure. Some conformational properties are discussed.

RX(202) OF 223 - 9 STEPS

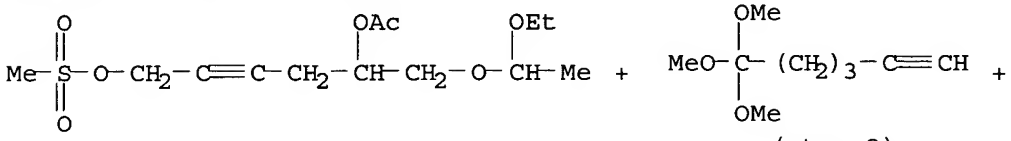


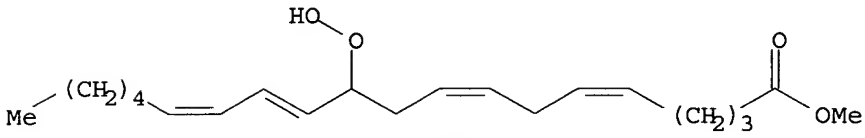




10%

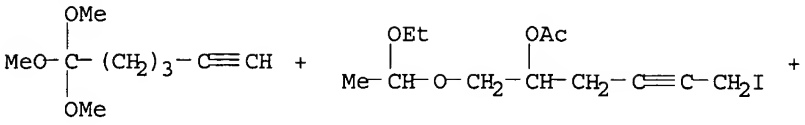
RX(204) OF 223 - 10 STEPS

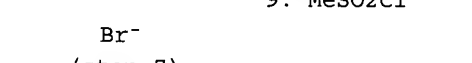


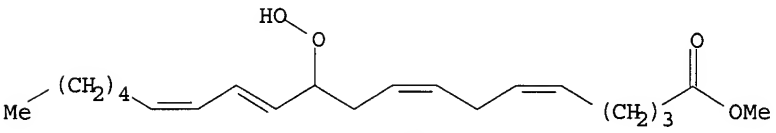


10%

RX(206) OF 223 - 10 STEPS

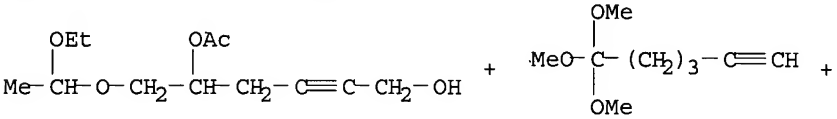




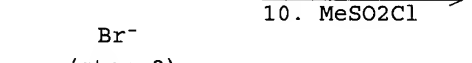


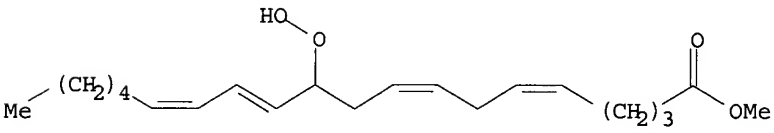
10%

RX(207) OF 223 - 11 STEPS



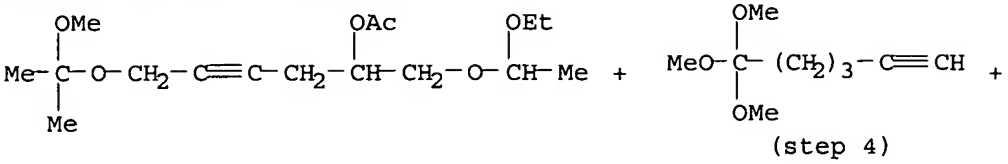
(step 3)



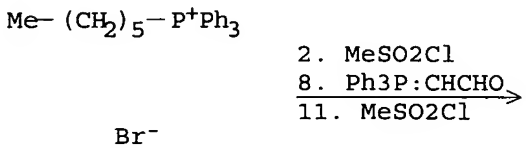


10%

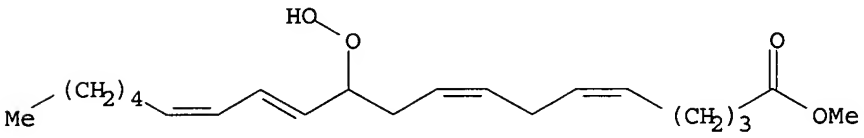
RX(208) OF 223 - 12 STEPS



(step 4)

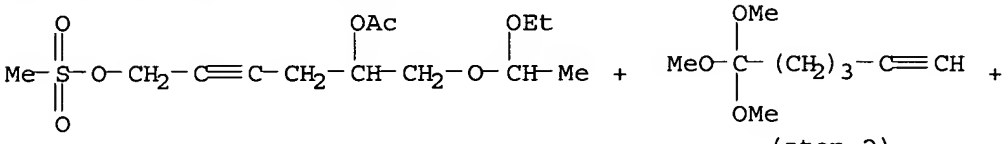


(step 9)



10%

RX(210) OF 223 - 11 STEPS



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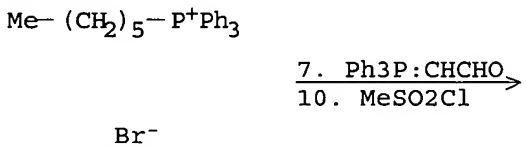
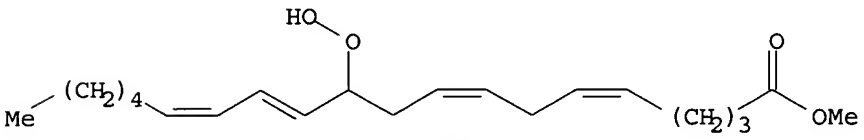


(step 8)



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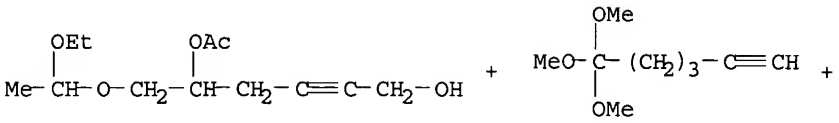
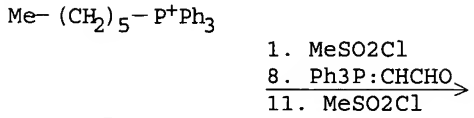
RX(212) OF 223 - 12 STEPS



(step 3)



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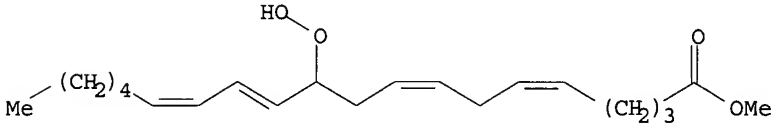

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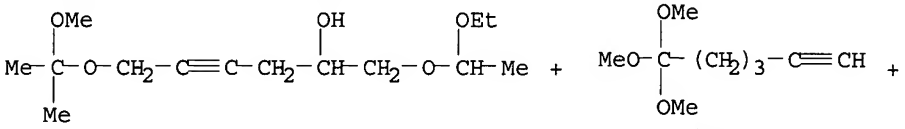
RX(213) OF 223 - 13 STEPS



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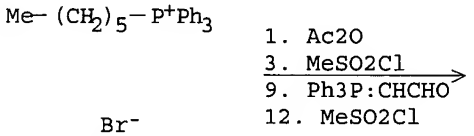
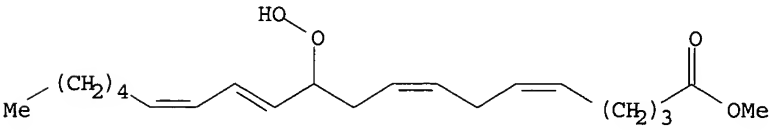


(step 10)



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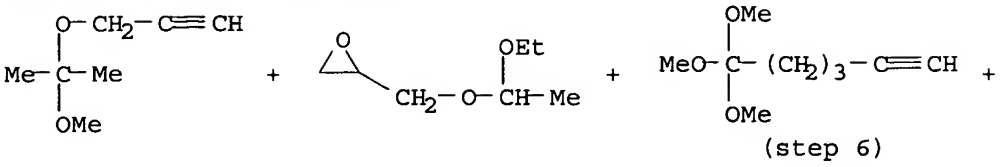
RX(214) OF 223 - 14 STEPS



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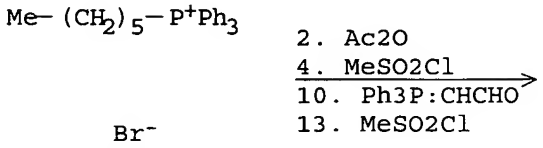
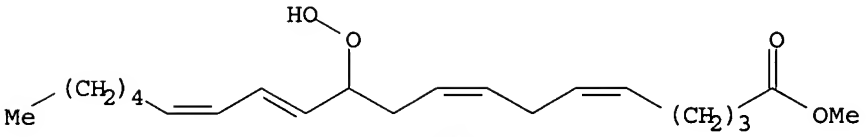
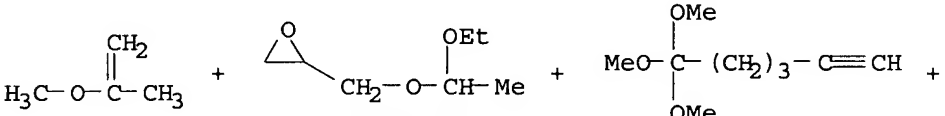


(step 11)



10%

RX(215) OF 223 - 15 STEPS



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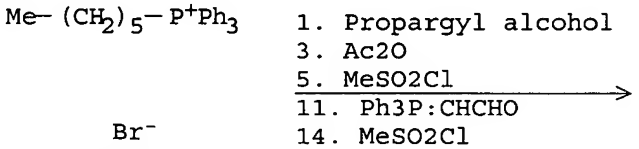

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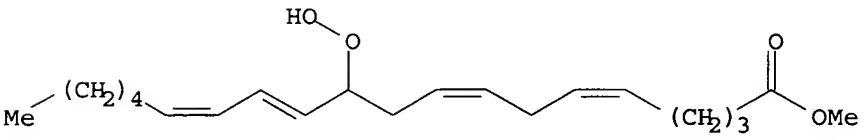

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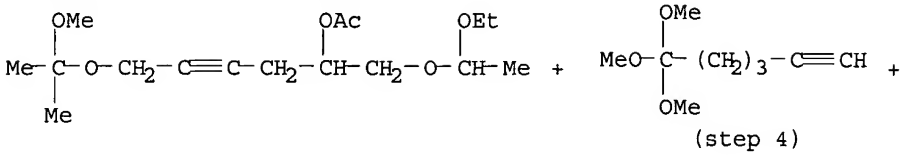
RX(217) OF 223 - 13 STEPS



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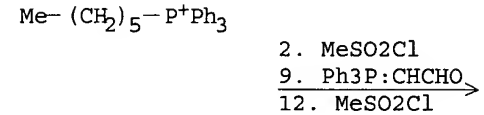

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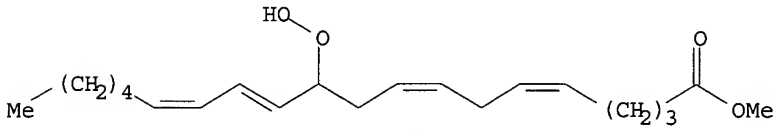

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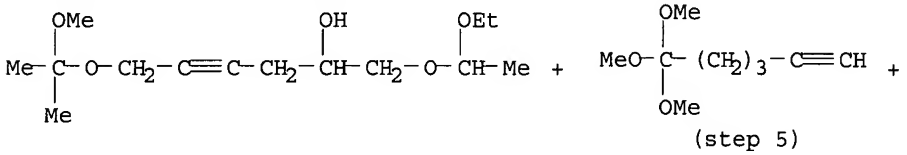
RX(219) OF 223 - 14 STEPS



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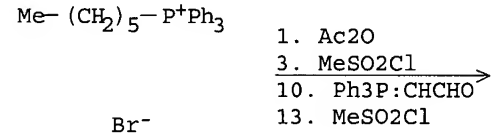

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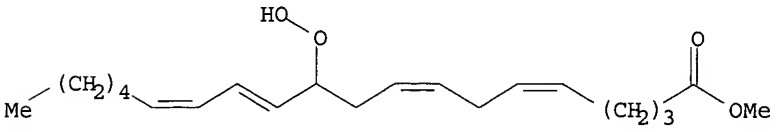

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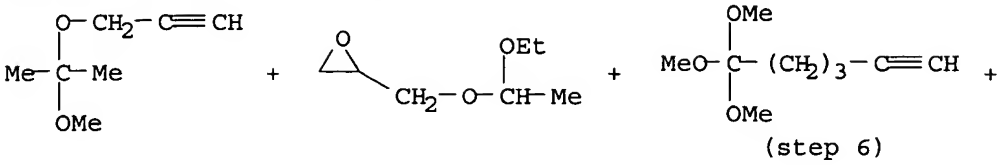
RX(221) OF 223 - 15 STEPS



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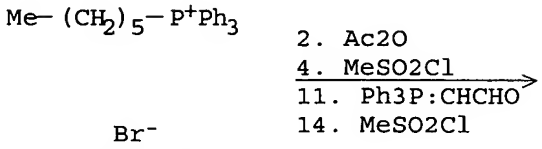
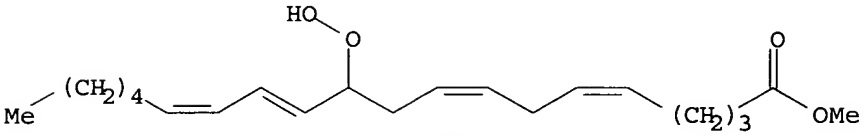


(step 12)



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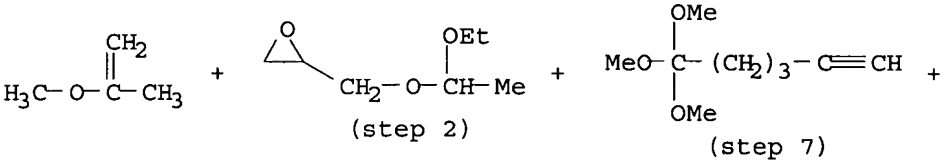
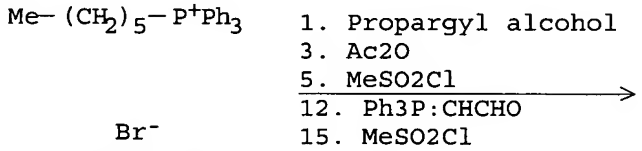
RX(223) OF 223 - 16 STEPS



(step 2) (step 7)



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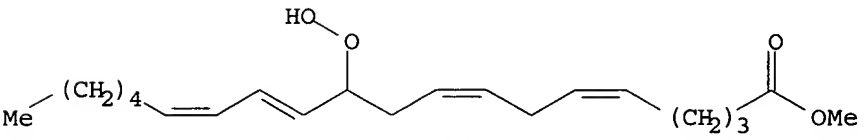
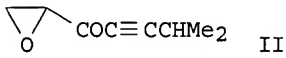


10%

L34 ANSWER 30 OF 76 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 93:167543 CASREACT
TITLE: Autoxidation of acetylenes. XXV. Products of the

autoxidation of 2-methyl-6-hepten-3-yne

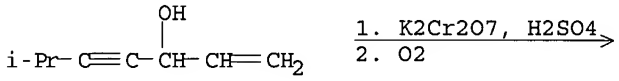
AUTHOR(S): Kudrevatykh, M. V.; Tishchenko, I. G.; Chirko, A. I.
CORPORATE SOURCE: Beloruss. Gos. Univ., Minsk, USSR
SOURCE: Vestsi Akademii Navuk BSSR, Seryya Khimichnykh Navuk (1980), (3), 110-14
CODEN: VBSKAK; ISSN: 0002-3590
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

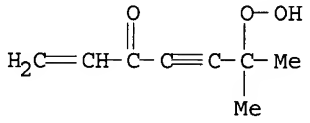


II

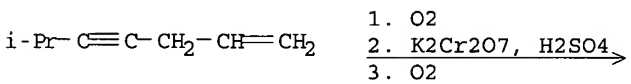
AB Grignard synthesis with CH2:CHCH2Br and HC.tplbond.CCHMe2 gave 80% CH2:CHCHXC:CCHMe2 (I; X = H), autoxidn. of which initially gave I (X = OOH) and CH2:CHCH2C.tplbond.CCMe2OOH. These decomposed to the corresponding alcs. Further oxidation of I (X = OOH) yielded the ketone, which was oxidized still further to give CH2:CHCOC.tplbond.CCMe2OOH and epoxide II.

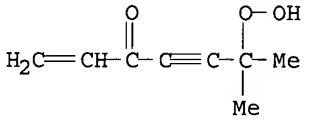
RX(21) OF 29 - 2 STEPS



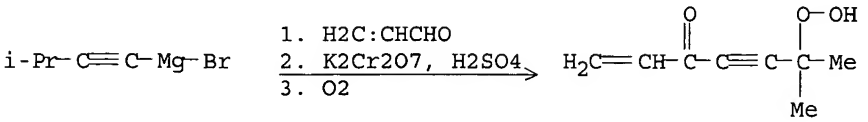


RX(25) OF 29 - 3 STEPS

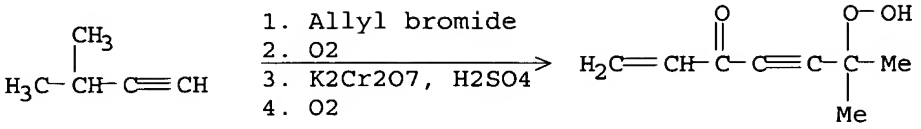




RX(27) OF 29 - 3 STEPS



RX(29) OF 29 - 4 STEPS



=> d l34 ibib abs hitstr 31-
YOU HAVE REQUESTED DATA FROM 46 ANSWERS - CONTINUE? Y/(N):y

L34 ANSWER 31 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:387846 CAPLUS
DOCUMENT NUMBER: 142:431972
TITLE: Process for the oxidation of cyclohexane
INVENTOR(S): Landray, David Paul; Fodor, Ludovic Rick; Murphree, Bruce Edwin; Rung, James Marvin
PATENT ASSIGNEE(S): Invista North America S.A.R.L., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6888034	B1	20050503	US 2003-702255	20031105
US 2005096486	A1	20050505		
WO 2005047243	A1	20050526	WO 2004-US36480	20041103

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-702255 A 20031105
OTHER SOURCE(S): CASREACT 142:431972

AB A process for oxidizing cyclohexane into cyclohexyl hydroperoxide, cyclohexanone, and cyclohexanol is described in which oxygen is contacted with cyclohexane at a pre-selected feed rate in a first reaction zone and unconsumed oxygen is contacted with cyclohexane in a second reaction zone in which the cyclohexane feed rate is lower than the pre-selected feed rate. Process flow diagrams are presented.

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(in a process for the oxidation of cyclohexane)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O═O

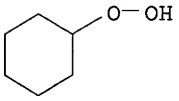
IT **7440-47-3**, Chromium, processes **7440-48-4**, Cobalt, processes
RL: **CAT (Catalyst use)**; EPR (Engineering process); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(oxidation **catalyst**; in a process for the oxidation of cyclohexane)
RN 7440-47-3 CAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7440-48-4 CAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: EPR (Engineering process); **IMF (Industrial manufacture)**; PEP (Physical, engineering or chemical process); **PREP (Preparation)**; PROC (Process)
(process for the oxidation of cyclohexane)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



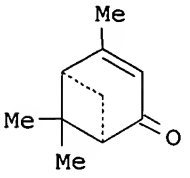
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 32 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:341550 CAPLUS
DOCUMENT NUMBER: 142:411505
TITLE: Method for the preparation of verbenone from α-pinene
INVENTOR(S): Frolova, L. L.; Kuchin, A. V.; Dreval, I. V.; Panteleeva, M. V.; Alekseev, I. N.
PATENT ASSIGNEE(S): Gosudarstvennoe Uchrezhdenie Institut Khimii Komi Nauchnogo Tsentra Ural'skogo Otdeleniya Rossiiskoi Akademii Nauk, Russia
SOURCE: Russ., No pp. given
CODEN: RUXXE7
DOCUMENT TYPE: Patent

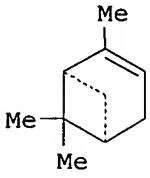
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RU 2250208	C2	20050420	RU 2003-121762	20030714
PRIORITY APPLN. INFO.:			RU 2003-121762	20030714

OTHER SOURCE(S): CASREACT 142:411505; MARPAT 142:411505
GI



I



II

AB Invention provides a method for preparation of verbenone (I), which is important intermediate in synthesis of perfumes, optically active insect pheromones and therapeutical prepns. Method involves catalytic oxidation of α-pinene (II) with air oxygen, wherein catalysts are selected from: a group including bivalent Cu, Zn, Pb, Co, Mn, and Ni (preferably Co, Mn, Ni), and Cr(III); a pyridine complex, M(C5H5N)2X2 [M represents bivalent transition metal, in particular, Co, Ni, and Mn; and X = halogen, e.g., Cl or Br]; or CrO3·M(C5H5N)2. Resulting hydroperoxides are then decomposed via fractioning steam distillation in alkali medium, wherein nonconverted α-pinene is separated at temperature below 97°C, whereas oxidized product fraction is distilled at 97-100°C and then subjected to addnl. oxidation with chromic mixture followed by recovering verbenone from addnl. oxidized products. Verbenone is further freed from myrtenal ingredient by reducing it into myrtenol with alkali metal borohydride in alc. or water-alc. solution, after which verbenone is recovered from reduction products.

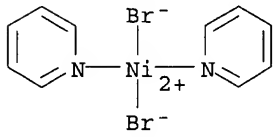
IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RGT (Reagent)**; **RACT (Reactant or reagent)**
(oxidation by, of α-pinene; preparation of verbenone from α-pinene via catalytic air oxidation)

RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

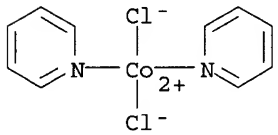
O=O

IT **14024-85-2 14024-92-1 14872-18-5**
20492-50-6, Dipyridinechromium trioxide **162635-76-9**, Chromium triseicosanoate
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation **catalyst**; preparation of verbenone from α-pinene via

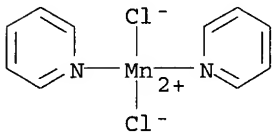
catalytic air oxidation)
RN 14024-85-2 CAPLUS
CN Nickel, dibromobis(pyridine)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



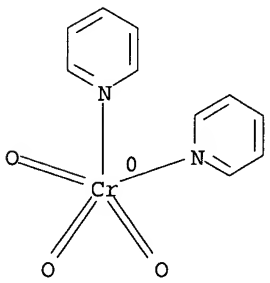
RN 14024-92-1 CAPLUS
CN Cobalt, dichlorobis(pyridine)-, (T-4)- (9CI) (CA INDEX NAME)



RN 14872-18-5 CAPLUS
CN Manganese, dichlorobis(pyridine)-, (T-4)- (9CI) (CA INDEX NAME)



RN 20492-50-6 CAPLUS
CN Chromium, trioxobis(pyridine)-, (TB-5-22)- (9CI) (CA INDEX NAME)



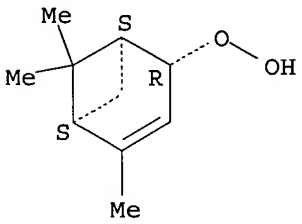
RN 162635-76-9 CAPLUS
CN Eicosanoic acid, chromium(3+) salt (9CI) (CA INDEX NAME)

$HO_2C-(CH_2)_{18}-Me$

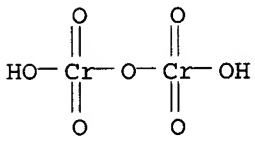
●1/3 Cr(III)

IT **850428-67-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and decomposition of, via fractioning steam distillation; preparation of
verbenone from α-pinene via catalytic air oxidation)
RN 850428-67-0 CAPLUS
CN Hydroperoxide, (1R,2S,5R)-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-yl, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **13530-68-2D**, Chromic acid, Jones reagent
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of verbenone from -pinene via **catalytic** air oxidation)
RN 13530-68-2 CAPLUS
CN Chromic acid (H2Cr2O7) (9CI) (CA INDEX NAME)



L34 ANSWER 33 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:317672 CAPLUS
DOCUMENT NUMBER: 142:489452
TITLE: Double channel electrode flow cell application to the study of HO2- production on MnxCo3-xO4 (0≤ x ≤1) spinel films
AUTHOR(S): Rios, E.; Reyes, H.; Ortiz, J.; Gautier, J. L.
CORPORATE SOURCE: Laboratorio de Electroquimica y Fisicoquimica de Solidos, Departamento de Quimica de los Materiales, Facultad de Quimica y Biologia, Universidad de Santiago de Chile, Santiago, 7254758, Chile
SOURCE: Electrochimica Acta (2005), 50(13), 2705-2711

CODEN: ELCAAV; ISSN: 0013-4686
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors conducted a study on the electroredn. of O2 in alkaline solution at room temperature on pure thin oxide electrodes MnxCo3-xO4 ($0 \leq x \leq 1$) using the double channel electrode flow cell (DCEFC). The oxides were prepared at 150° and deposited by spray pyrolysis onto Ti substrates. The oxygen reduction reaction (orr) occurs through interactive and parallel pathways, and the ratio of O2 mols. reduced to OH- ions with respect to those reduced to HO2- ions depends on the oxide stoichiometry and on the applied overpotential. The formation of HO2- increases when the Mn concentration increases. The results obtained for the orr show that the number of electrons transferred per O2 mol. decreases from 3 to 2 and the ratio k1/k2 (the rate consts. for direct reduction to OH- and indirect reduction to HO2-) increases, resp., in the overpotential studied range (-0.05 to -0.6 V). The Mn3+ ions placed in the B-sites of the spinel structure seem to be the active centers, where H2O2 is formed.

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(electrochem. reduction on MnxCo3-xO4 ($0 \leq x \leq 1$) spinel films in double channel electrode flow cell in HO2- production)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O═O

IT **452976-56-6**, Cobalt manganese oxide (Co2-3Mn0-1O4)
RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
(oxygen electrochem. reduction on MnxCo3-xO4 ($0 \leq x \leq 1$) spinel films in double channel electrode flow cell in HO2- production)
RN 452976-56-6 CAPLUS
CN Cobalt manganese oxide (Co2-3Mn0-1O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2 - 3	7440-48-4
Mn	0 - 1	7439-96-5

IT **14691-59-9P**, Peroxide (HO21-)
RL: **PNU (Preparation, unclassified)**; **PREP (Preparation)**
(oxygen electrochem. reduction on MnxCo3-xO4 ($0 \leq x \leq 1$) spinel films in double channel electrode flow cell in HO2- production)
RN 14691-59-9 CAPLUS
CN Peroxide (HO21-) (8CI, 9CI) (CA INDEX NAME)

$^{-}$O—OH

IT **1308-06-1**, Cobalt oxide (Co3O4) **12139-92-3**, Cobalt manganese oxide (Co2MnO4) **183864-63-3**, Cobalt manganese oxide

(Co2.75Mn0.25O4) **183864-65-5**, Cobalt manganese oxide
(Co2.5Mn0.5O4) **183864-67-7**, Cobalt manganese oxide
(Co2.25Mn0.75O4)
RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
(oxygen electrochem. reduction on cobalt oxide and cobalt manganese oxide spinel films in double channel electrode flow cell in HO2- production)
RN 1308-06-1 CAPLUS
CN Cobalt oxide (Co3O4) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 12139-92-3 CAPLUS
CN Cobalt manganese oxide (Co2MnO4) (6CI, 9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2	7440-48-4
Mn	1	7439-96-5

RN 183864-63-3 CAPLUS
CN Cobalt manganese oxide (Co2.75Mn0.25O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2.75	7440-48-4
Mn	0.25	7439-96-5

RN 183864-65-5 CAPLUS
CN Cobalt manganese oxide (Co2.5Mn0.5O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2.5	7440-48-4
Mn	0.5	7439-96-5

RN 183864-67-7 CAPLUS
CN Cobalt manganese oxide (Co2.25Mn0.75O4) (9CI) (CA INDEX NAME)

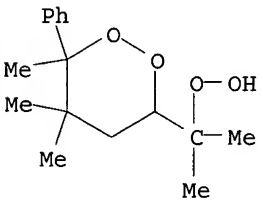
Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2.25	7440-48-4
Mn	0.75	7439-96-5

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

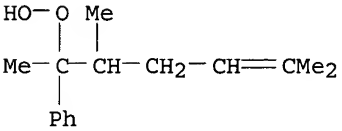
L34 ANSWER 34 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1052421 CAPLUS
DOCUMENT NUMBER: 142:155918
TITLE: Synthesis of Cyclic Peroxides by Chemo- and Regioselective Peroxidation of Dienes with Co(II)/O2/Et3SiH

AUTHOR(S): Tokuyasu, Takahiro; Kunikawa, Shigeki; McCullough, Kevin J.; Masuyama, Araki; Nojima, Masatomo
CORPORATE SOURCE: Department of Materials Chemistry, Frontier Research Center, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan
SOURCE: Journal of Organic Chemistry (2005), 70(1), 251-260
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the competitive peroxidn. of mixts. of two alkenes with Co(II)/O2/Et3SiH, it was found that the relative reactivities of the alkene substrates are influenced by three major factors: relative stability of the intermediate carbon-centered radical formed by the reaction of the alkene with HCo(III) complex, steric effects around the carbon-carbon double bond, and electronic factors associated with the carbon-carbon double bond. Consistent with results from simple alkenes, the chemoselective and regioselective peroxidn. of dienes was also realized. Depending on the diene structure, the product included not only the expected acyclic unsatd. triethylsilyl peroxides but also 1,2-dioxolane and 1,2-dioxane derivs. via intramol. cyclization of the unsatd. peroxy radical intermediates.

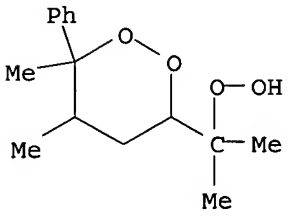
IT **830345-40-9P**
RL: PRP (Properties); **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of [(1,2-dioxanyl)methyl]hydroperoxide and study of its crystal and mol. structures)
RN 830345-40-9 CAPLUS
CN Hydroperoxide, 1-methyl-1-(5,5,6-trimethyl-6-phenyl-1,2-dioxan-3-yl)ethyl (9CI) (CA INDEX NAME)



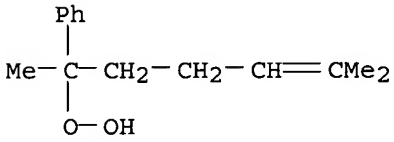
IT **830345-32-9P 830345-33-0P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of cyclic peroxides, dioxane derivs. and silyl peroxides by chemoselective, regioselective peroxidn. of [dimethyl(methylene)hexenyl]benzene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-32-9 CAPLUS
CN Hydroperoxide, 1,2,5-trimethyl-1-phenyl-4-hexenyl (9CI) (CA INDEX NAME)



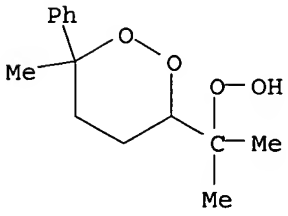
RN 830345-33-0 CAPLUS
CN Hydroperoxide, 1-(5,6-dimethyl-6-phenyl-1,2-dioxan-3-yl)-1-methylethyl (9CI) (CA INDEX NAME)



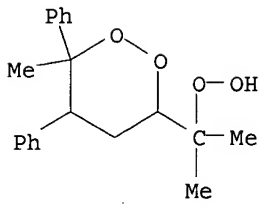
IT **830345-29-4P 830345-30-7P 830345-38-5P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of cyclic peroxides, dioxane derivs. and silyl peroxides by chemoselective, regioselective peroxidn. of [methyl(methylene)hexenyl]benzene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-29-4 CAPLUS
CN Hydroperoxide, 1,5-dimethyl-1-phenyl-4-hexenyl (9CI) (CA INDEX NAME)



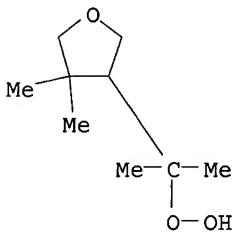
RN 830345-30-7 CAPLUS
CN Hydroperoxide, 1-methyl-1-(6-methyl-6-phenyl-1,2-dioxan-3-yl)ethyl (9CI) (CA INDEX NAME)



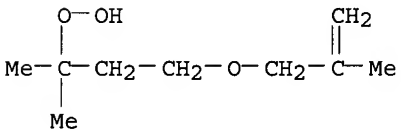
RN 830345-38-5 CAPLUS
CN Hydroperoxide, 1-methyl-1-(6-methyl-5,6-diphenyl-1,2-dioxan-3-yl)ethyl (9CI) (CA INDEX NAME)



IT **830345-55-6P 830345-56-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by chemoselective, regioselective peroxidn. of (methyl)[[(methyl)propenyl]oxy]butene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-55-6 CAPLUS
CN Hydroperoxide, 1-methyl-1-(tetrahydro-4,4-dimethyl-3-furanyl)ethyl (9CI) (CA INDEX NAME)

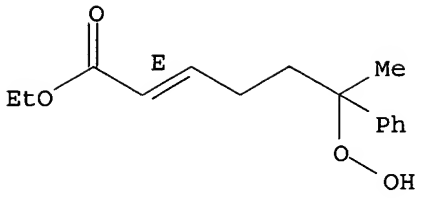


RN 830345-56-7 CAPLUS
CN Hydroperoxide, 1,1-dimethyl-3-[(2-methyl-2-propenyl)oxy]propyl (9CI) (CA INDEX NAME)

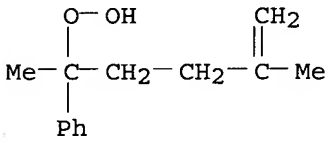


IT **830345-51-2P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by chemoselective, regioselective peroxidn. of (phenyl)heptadienoic acid ester using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-51-2 CAPLUS
CN 2-Heptenoic acid, 6-hydroperoxy-6-phenyl-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

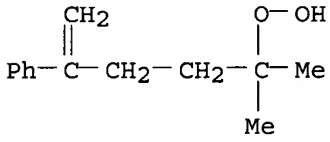
Double bond geometry as shown.



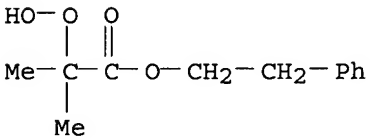
IT **830345-48-7P 830345-49-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by chemoselective, regioselective peroxidn. of [(methyl)(methylene)pentenyl]benzene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-48-7 CAPLUS
CN Hydroperoxide, 1,4-dimethyl-1-phenyl-4-pentenyl (9CI) (CA INDEX NAME)



RN 830345-49-8 CAPLUS
CN Hydroperoxide, 1,1-dimethyl-4-phenyl-4-pentenyl (9CI) (CA INDEX NAME)



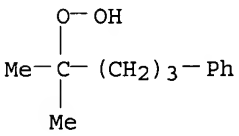
IT **830345-67-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by chemoselective, regioselective peroxidn. of alkene using bis[[di(methyl)di(oxo-O)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system and study of influence of electronic effects on product formation)
RN 830345-67-0 CAPLUS
CN Propanoic acid, 2-hydroperoxy-2-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



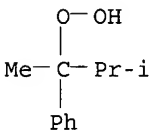
IT **34586-03-3P 42238-03-9P 42805-25-4P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by chemoselective, regioselective peroxidn. of alkene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system and study of influence of steric congestion on product formation)

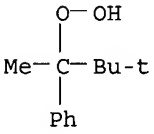
RN 34586-03-3 CAPLUS
CN Hydroperoxide, 1,1-dimethyl-4-phenylbutyl (9CI) (CA INDEX NAME)



RN 42238-03-9 CAPLUS
CN Hydroperoxide, 1,2-dimethyl-1-phenylpropyl (9CI) (CA INDEX NAME)

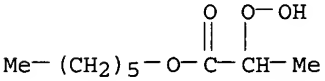


RN 42805-25-4 CAPLUS
CN Hydroperoxide, 1,2,2-trimethyl-1-phenylpropyl (9CI) (CA INDEX NAME)



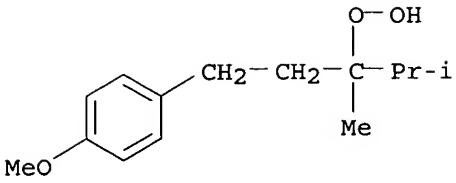
IT **830345-69-2P 830345-71-6P 830345-73-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of peroxide by peroxidn. of alkene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane and study of influence of relative stability of radical intermediates on product formation)

RN 830345-69-2 CAPLUS
CN Propanoic acid, 2-hydroperoxy-, hexyl ester (9CI) (CA INDEX NAME)

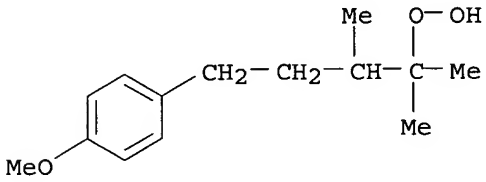


RN 830345-71-6 CAPLUS
CN Hydroperoxide, 1-[2-(4-methoxyphenyl)ethyl]-1,2-dimethylpropyl (9CI) (CA

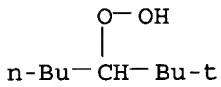
INDEX NAME)



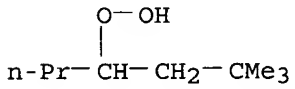
RN 830345-73-8 CAPLUS
CN Hydroperoxide, 4-(4-methoxyphenyl)-1,1,2-trimethylbutyl (9CI) (CA INDEX NAME)



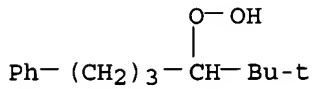
IT **830345-79-4P 830345-81-8P 830345-83-0P**
830345-85-2P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of peroxide by peroxidn. of alkene using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system and study of influence of relative reactivity on product formation)
RN 830345-79-4 CAPLUS
CN Hydroperoxide, 1-(1,1-dimethylethyl)pentyl (9CI) (CA INDEX NAME)



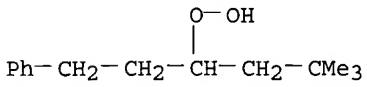
RN 830345-81-8 CAPLUS
CN Hydroperoxide, 3,3-dimethyl-1-propylbutyl (9CI) (CA INDEX NAME)



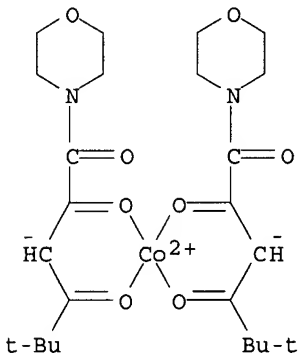
RN 830345-83-0 CAPLUS
CN Hydroperoxide, 1-(1,1-dimethylethyl)-4-phenylbutyl (9CI) (CA INDEX NAME)



RN 830345-85-2 CAPLUS
CN Hydroperoxide, 3,3-dimethyl-1-(2-phenylethyl)butyl (9CI) (CA INDEX NAME)

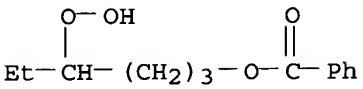


IT **124027-94-7**, Bis(1-morpholinocarbamoyl-4,4-dimethyl-1,3-pentanedionato)cobalt(II)
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of peroxides by chemoselective, regioselective peroxidn. of dienes using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 124027-94-7 CAPLUS
CN Cobalt, bis[4-[5,5-dimethyl-2,4-di(oxo-κO)-1-oxohexyl]morpholinato]-(9CI) (CA INDEX NAME)

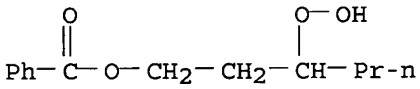


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of peroxides by chemoselective, regioselective peroxidn. of dienes using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

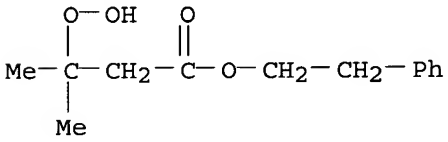
IT **830345-26-1P 830345-27-2P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(study of peroxidn. of (Z)-hexenol benzoate using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane system)
RN 830345-26-1 CAPLUS
CN 1-Hexanol, 4-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



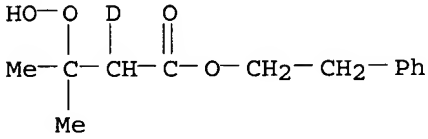
RN 830345-27-2 CAPLUS
CN 1-Hexanol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



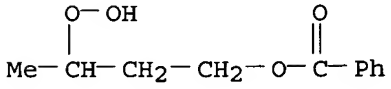
IT **830345-24-9P 830345-25-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(study of peroxidn. of (methyl)butenoic acid phenylethyl ester using bis[[di(methyl)di(oxo-κO)-(oxo)hexyl]morpholinato]cobalt/oxygen/triethylsilane-d system)
RN 830345-24-9 CAPLUS
CN Butanoic acid, 3-hydroperoxy-3-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



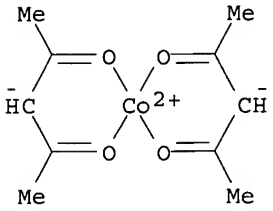
RN 830345-25-0 CAPLUS
CN Butanoic-2-d acid, 3-hydroperoxy-3-methyl-, 2-phenylethyl ester (9CI) (CA INDEX NAME)



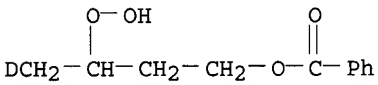
IT **830345-65-8P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(study of peroxidn. of butenol benzoate using bis(pentanedionato)cobalt/oxygen/triethylsilane system)
RN 830345-65-8 CAPLUS
CN 1-Butanol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



IT **14024-48-7**, Bis(acetylacetonato)cobalt
RL: **CAT (Catalyst use)**; USES (Uses)
(study of peroxidn. of butenol benzoate using bis(pentanedionato)cobalt/oxygen/triethylsilane-d system)
RN 14024-48-7 CAPLUS
CN Cobalt, bis(2,4-pentanedionato-κO,κO')-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT **830345-28-3P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(study of peroxidn. of butenol benzoate using bis(pentanedionato)cobalt/oxygen/triethylsilane-d system)
RN 830345-28-3 CAPLUS
CN 1-Butan-4-d-ol, 3-hydroperoxy-, benzoate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 35 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:817834 CAPLUS
DOCUMENT NUMBER: 141:316241
TITLE: Process for the catalytic hydrogenation of alkylaryl ketones in the presence of phenolic compounds
INVENTOR(S): Nisbet, Timothy Michael; Van Zwienen, Marinus
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004085354	A2	20041007	WO 2004-EP50362	20040325
WO 2004085354	A3	20050317		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

US 2004220431 A1 20041104 US 2004-808858 20040325
PRIORITY APPLN. INFO.: EP 2003-251987 A 20030328

AB A process for the catalytic hydrogenation of alkylaryl ketones (e.g., acetophenone) into their corresponding alcs. (e.g., 1-phenyl-1-ethanol) comprises contacting a feed comprising the alkylaryl ketones and 0.5-30% of phenolic compds. (e.g., phenol) with hydrogen in the presence of a heterogeneous hydrogenation catalyst (e.g., copper). A process for preparing a hydrogenation catalyst with improved activity, and to the use of phenolic compds. for the activation of the hydrogenation catalysts is described.

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of alkylaryl compds. with)

RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **7440-50-8**, Copper, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(process for the **catalytic** hydrogenation of alkylaryl ketones in the presence of phenolic compds.)

RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 36 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:261000 CAPLUS
DOCUMENT NUMBER: 140:287556
TITLE: Process for singlet oxygen oxidation of organic substrates
INVENTOR(S): Emsenhuber, Martin; Kwant, Gerard; Van Straaten, Koenraad; Janssen, Madelon; Alsters, Paul; Hoving, Hendrik
PATENT ASSIGNEE(S): DSM Fine Chemicals Austria Nfg G.m.b.H. & Co. K.-G., Austria
SOURCE: Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1403234	A2	20040331	EP 2003-19797	20030830
EP 1403234	A3	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 200201443	A5	20050415	AT 2002-1443	20020926
US 2004220416	A1	20041104	US 2003-668259	20030924
JP 2004137269	A2	20040513	JP 2003-334055	20030925
PRIORITY APPLN. INFO.:			AT 2002-1443 A	20020926

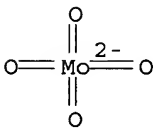
OTHER SOURCE(S): CASREACT 140:287556

AB Improved procedure for the oxidation of organic substrates, especially olefins [1 - 10 double bonds, (un)substituted C6-30-aroms., polyaroms. (2 - 8 rings), alkylsulfides, alkenylsulfides, arylsulfides, C4-30-heterocyclics (with 1 or more O, N, S); substituted with halogen, CN, :CO, OH, C1-20-alkoxy, C1-20-alkyl, C6-30-aryl, C2-20-alkenyl, C2-20-alkynyl, CO2H, ester, amide, NH2, NO2, silyl, siloxy, sulfono, sulfoxo, NR1R2; R1, R2 = H, C1-20-alkyl, CHO, C2-20-acyl, C7-30-benzoyl; R1R2 = ring], with singlet oxygen is characterized by reaction of the organic substrate with 1O2 in H2O or an aqueous solution of a water miscible organic solvent in the presence of a heterogeneous or homogeneous catalyst and aqueous H2O2 whereby the catalyst decompses the H2O2 to 1O2 and water is removed from the reaction by a water selective membrane. Thus, β-citronellol in an aqueous methanol solution containing catalytic Na2MoO4 is treated with aqueous H2O2 whereby the solution is pumped past a membrane separating out the H2O. Water removal with a pervaporation membrane was tested with a test solution containing sodium tiglate in aqueous MeOH. Process schematics are provided.

IT **7631-95-0**, Sodium molybdate
RL: **CAT (Catalyst use)**; USES (Uses)
(decomposition **catalyst**; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)

RN 7631-95-0 CAPLUS

CN Molybdate (MoO42-), disodium, (T-4)- (9CI) (CA INDEX NAME)



●2 Na+

IT **7439-98-7D**, Molybdenum, compds. **7440-62-2D**, Vanadium, compds.
RL: **CAT (Catalyst use)**; USES (Uses)
(decomposition **catalysts**; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)

RN 7439-98-7 CAPLUS

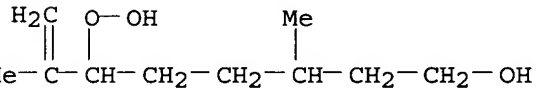
CN Molybdenum (8CI, 9CI) (CA INDEX NAME)

Mo

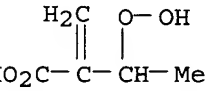
RN 7440-62-2 CAPLUS
CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

IT **81113-74-8P 99268-55-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by a water selective membrane)
RN 81113-74-8 CAPLUS
CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 99268-55-0 CAPLUS
CN Butanoic acid, 3-hydroperoxy-2-methylene- (9CI) (CA INDEX NAME)



IT **7782-44-7D**, Oxygen, singlet
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, with citronellol and tiglate; process for singlet oxygen oxidation of organic substrates whereby water is removed from the reaction by
a water selective membrane)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

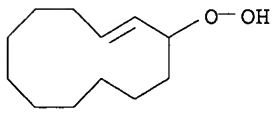
L34 ANSWER 37 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:431670 CAPLUS
DOCUMENT NUMBER: 141:125349
TITLE: Uncatalyzed Liquid-Phase Oxidation of Cyclododecene with Molecular Oxygen
AUTHOR(S): Mahajan, S. S.; Sharma, M. M.; Sridhar, T.

CORPORATE SOURCE: Department of Chemical Engineering, Monash University, Victoria, 3800, Australia
SOURCE: Industrial & Engineering Chemistry Research (2004), 43(13), 3289-3296
CODEN: IECRED; ISSN: 0888-5885
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:125349

AB Uncatalyzed liquid-phase oxidation of cyclododecene was studied in a batch reactor. Cyclododecene was oxidized with mol. oxygen at of 363-383 K. Cyclododecene oxide, cyclododecene hydroperoxide, and cyclododecenol were obtained as reaction products. The oxidation kinetics were studied in detail, and a mechanism was devised based on the exptl. results and existing literature. The kinetic data were generated at different reaction parameters and fitted successfully with a rate equation based on autocatalysis by total products. The values of the reaction rate consts. and activation energy were determined A distinct difference was observed between the reaction rates of the cis and trans isomers of cyclododecene. The oxidation kinetics were also studied in a stainless steel reactor to examine the catalytic effect on reactivity of cyclododecene; no difference was observed vs. glass wall reactors. The presence of metal ions was found to affect the product distribution.

IT **7782-44-7**, Oxygen, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(kinetics and mechanism of uncatalyzed liquid-phase oxidation of cyclododecene with mol. oxygen)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **723308-17-6P**, Cyclododecene hydroperoxide
RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**
(kinetics and mechanism of uncatalyzed liquid-phase oxidation of cyclododecene with mol. oxygen)
RN 723308-17-6 CAPLUS
CN Hydroperoxide, 2-cyclododecen-1-yl (9CI) (CA INDEX NAME)



IT **11107-04-3**, SS 316
RL: DEV (Device component use); USES (Uses)
(reactor; kinetics and mechanism of **uncatalyzed** liquid-phase oxidation of cyclododecene with mol. oxygen)
RN 11107-04-3 CAPLUS
CN Iron alloy, base, Fe 62-72,Cr 16.00-18.00,Ni 10.00-14.00,Mo 2.00-3.00,Mn

0-2.00,Si 0-1.00,C 0-0.08,P 0-0.045,S 0-0.030 (UNS S31600) (9CI) (CA INDEX NAME)

Component	Component Percent	Component Registry Number
Fe	62 - 72	7439-89-6
Cr	16.00 - 18.00	7440-47-3
Ni	10.00 - 14.00	7440-02-0
Mo	2.00 - 3.00	7439-98-7
Mn	0 - 2.00	7439-96-5
Si	0 - 1.00	7440-21-3
C	0 - 0.08	7440-44-0
P	0 - 0.045	7723-14-0
S	0 - 0.030	7704-34-9

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

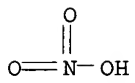
L34 ANSWER 38 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:166974 CAPLUS
DOCUMENT NUMBER: 138:221456
TITLE: Preparation of olefin oxidation products using heteropoly acid catalysts
INVENTOR(S): Furuya, Masahiko; Nakashima, Hitoshi
PATENT ASSIGNEE(S): Asahi Kasei Corporation, Japan; Noguchi Research Institute
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003064007	A2	20030305	JP 2001-258538	20010828
PRIORITY APPLN. INFO.:			JP 2001-258538	20010828

AB The products are prepared by oxidation of olefins by mol. O in the presence of heteropoly acid catalysts containing rare earth elements, Group IVB, VB, VIB, or VIIB elements, Ni, Pd, Ir, or Pt in their double defects. Cyclooctene was oxidized by O in dichloroethane-MeCN mixture in the presence of Y-substituted tetrabutylammonium tungstosilicate (preparation given) at 75° for 75 h to give cyclooctene oxide with 86% selectivity at 20% conversion.

IT **13138-45-9DP**, Nickel dinitrate, reaction products with decatungstosilicic acid and tetrabutylammonium nitrate
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(**catalyst**; preparation of olefin oxidation products using heteropoly acid **catalysts**)

RN 13138-45-9 CAPLUS
CN Nitric acid, nickel(2+) salt (8CI, 9CI) (CA INDEX NAME)



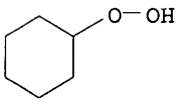
●1/2 Ni(II)

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(mol.; preparation of olefin oxidation products using heteropoly acid catalysts)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **27254-23-5P**, Cyclohexenyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of olefin oxidation products using heteropoly acid catalysts)
RN 27254-23-5 CAPLUS
CN Hydroperoxide, cyclohexenyl (9CI) (CA INDEX NAME)

CM 1

CRN 766-07-4
CMF C6 H12 O2



L34 ANSWER 39 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:791395 CAPLUS
DOCUMENT NUMBER: 139:291994
TITLE: Method and cobalt-ruthenium catalyst systems for oxidizing cycloalkanes into cycloalkanols and cycloalkanones and hydroperoxycycloalkanes
INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo
PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan
SOURCE: Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 1350783	A1	20031008	EP 2003-7537	20030401
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004002327	A2	20040108	JP 2003-77387	20030320
US 2003216601	A1	20031120	US 2003-396832	20030326
CN 1448378	A	20031015	CN 2003-121238	20030328

PRIORITY APPLN. INFO.: JP 2002-101001 A 20020403
OTHER SOURCE(S): CASREACT 139:291994
AB A method for producing an oxygenated compound (e.g., cyclohexanol and mixts. of cyclohexanone and cyclohexyl hydroperoxide) from a cycloalkane (e.g., cyclohexane) is characterized in that the cycloalkane is contacted with oxygen in the presence of a cobalt compound [e.g., cobalt(II) octylate] and a ruthenium compound [e.g., ruthenium(III) acetylacetonate].
IT **1588-79-0**, CobaltII octanoate **7440-48-4**, Cobalt, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(method and cobalt-ruthenium **catalyst** systems for oxidizing cycloalkanes into cycloalkanols and cycloalkanones and hydroperoxycycloalkanes)
RN 1588-79-0 CAPLUS
CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

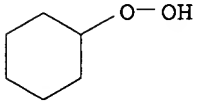
$HO_2C-(CH_2)_6-Me$

●1/2 Co(II)

RN 7440-48-4 CAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(method and cobalt-ruthenium catalyst systems for oxidizing cycloalkanes into cycloalkanols and cycloalkanones and hydroperoxycycloalkanes)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(method and cobalt-ruthenium catalyst systems for oxidizing cycloalkanes into cycloalkanols and cycloalkanones and

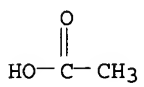
hydroperoxycycloalkanes using)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

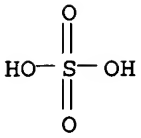
L34 ANSWER 40 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:458023 CAPLUS
DOCUMENT NUMBER: 142:96308
TITLE: Method for preparing cyclohexanone and cyclohexanol from cyclohexane
INVENTOR(S): Zhou, Xiaowen; Liu, Jihong; Yin, Huaqing; Hu, Xuewu; Li, Juan
PATENT ASSIGNEE(S): Yueyang Petro-Chemical General Plant, Baling Petro-Chemical Co., Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 11 pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1397538	A	20030219	CN 2001-114586	20010713
PRIORITY APPLN. INFO.:			CN 2001-114586	20010713

AB A method comprises oxidizing cyclohexane with an O-containing gas to obtain cyclohexyl hydroperoxide-containing mixts., decomposing with aqueous Na2CO3 solns. optionally containing Na carboxylates in the presence of 0.1-100 ppm soluble transition metal salt (such as Co sulfate or Co acetate) catalysts at 60°-120° and 100-1,200 kPa, decomposing again with aqueous NaOH solns. optionally containing Na carboxylates in the presence of 0.1-10 ppm soluble transition metal salts at 100-1,200 kPa, and distilling
IT **5931-89-5**, Cobalt acetate **10124-43-3**, Cobalt sulfate
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)
RN 5931-89-5 CAPLUS
CN Acetic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)

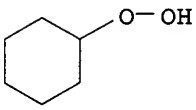


RN 10124-43-3 CAPLUS
CN Sulfuric acid, cobalt(2+) salt (1:1) (8CI, 9CI) (CA INDEX NAME)



● Co(II)

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture)**; RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of cyclohexane for manufacture of cyclohexanone and cyclohexanol)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

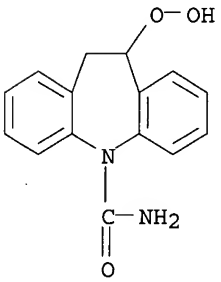
L34 ANSWER 41 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:109222 CAPLUS
DOCUMENT NUMBER: 139:22104
TITLE: Low temperature, high conversion, liquid-phase benzylic oxidation with dioxygen by metal/NHPI-catalyzed Co-oxidation with benzaldehyde
AUTHOR(S): Schmieder-van de Vondervoort, Lizette; Bouttemy, Sabine; Heu, Ferdinand; Weissenbock, Kurt; Alsters, Paul L.
CORPORATE SOURCE: Advanced Synthesis and Catalysis, DSM Fine Chemicals, Geleen, 6160 MD, Neth.
SOURCE: European Journal of Organic Chemistry (2003), (3), 578-586
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:22104

AB A new liquid-phase catalytic oxidation system for the low temperature, high conversion benzylic mono-oxyfunctionalization of 5H-dibenz[b,f]azepine-5-carboxamide (I) into oxcarbazepine with dioxygen has been developed. The method is based on a co-oxidation of I with benzaldehyde in the presence of a four-component catalyst system consisting of Co(OAc)2, Ni(OAc)2, Cr(NO3)3, and N-hydroxyphthalimide (NHPI). The influence of the catalyst system on the formation and decomposition of the crucial hydroperoxide intermediate has been investigated. Based on these results, the role of each of the components in the catalyst system is discussed. The scope of this method for the oxidation of other substrates has been studied, and the results are compared with those obtained by Co/NHPI catalyzed oxidation of these substrates.

IT **537693-28-0P**, 10,11-Dihydro-10-hydroperoxy-5H-dibenz[b,f]azepine-5-carboxamide
RL: **BYP (Byproduct)**; RCT (Reactant); **PREP (Preparation)**
; RACT (Reactant or reagent)
(low temperature, high-conversion, liquid-phase oxidation of 5H-dibenz[b,f]azepine-
5-carboxamide with dioxygen in presence of metal/N-hydroxyphthalimide catalyst and benzaldehyde)

RN 537693-28-0 CAPLUS

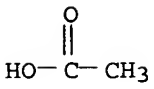
CN 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-10-hydroperoxy- (9CI) (CA INDEX NAME)



IT **71-48-7**, Acetic acid cobalt(2+) salt **142-71-2**, Acetic acid copper(2+) salt **373-02-4**, Acetic acid nickel(2+) salt **638-38-0**, Acetic acid manganese(2+) salt **1313-27-5**, Molybdenum oxide (MoO3), uses **3094-87-9**, Acetic acid iron(2+) salt **3264-82-2**, Bis(acetylacetonato)nickel **7718-54-9**, Nickel chloride (NiCl2), uses **13476-99-8**, Tris(acetylacetonato)vanadium **13548-38-4**, Chromium nitrate [Cr(NO3)3] **21679-31-2**, Tris(acetylacetonato)chromium
RL: **CAT (Catalyst use)**; USES (Uses)
(low temperature, high-conversion, liquid-phase oxidation of benzylic compds. with dioxygen in presence of metal/N-hydroxyphthalimide **catalyst** and benzaldehyde)

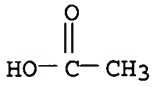
RN 71-48-7 CAPLUS

CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



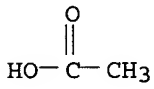
●1/2 Co(II)

RN 142-71-2 CAPLUS
CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)



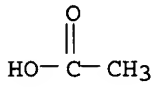
●1/2 Cu(II)

RN 373-02-4 CAPLUS
CN Acetic acid, nickel(2+) salt (8CI, 9CI) (CA INDEX NAME)



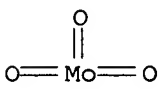
●1/2 Ni(II)

RN 638-38-0 CAPLUS
CN Acetic acid, manganese(2+) salt (8CI, 9CI) (CA INDEX NAME)

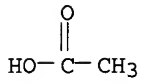


●1/2 Mn(II)

RN 1313-27-5 CAPLUS
CN Molybdenum oxide (MoO3) (7CI, 8CI, 9CI) (CA INDEX NAME)

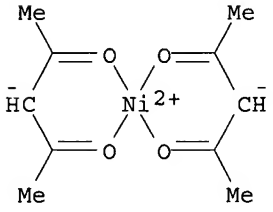


RN 3094-87-9 CAPLUS
CN Acetic acid, iron(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Fe(II)

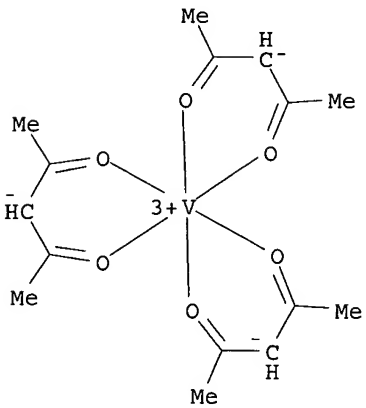
RN 3264-82-2 CAPLUS
CN Nickel, bis(2,4-pentanedionato-κO,κO')-, (SP-4-1)- (9CI) (CA INDEX NAME)



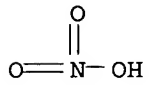
RN 7718-54-9 CAPLUS
CN Nickel chloride (NiCl2) (8CI, 9CI) (CA INDEX NAME)

Cl—Ni—Cl

RN 13476-99-8 CAPLUS
CN Vanadium, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI) (CA INDEX NAME)

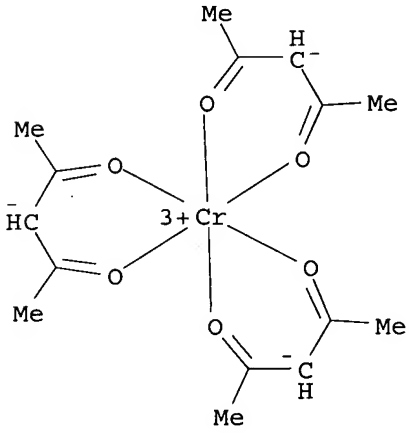


RN 13548-38-4 CAPLUS
CN Nitric acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)



●1/3 Cr(III)

RN 21679-31-2 CAPLUS
CN Chromium, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



IT **7782-44-7**, Dioxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(low temperature, high-conversion, liquid-phase oxidation of benzylic compds. with
dioxygen in presence of metal/N-hydroxyphthalimide catalyst and benzaldehyde)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 42 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:290164 CAPLUS
DOCUMENT NUMBER: 139:133158
TITLE: Selective Oxidation of Ethylbenzene by Molecular

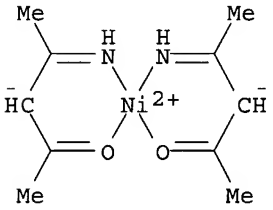
Oxygen: Effect of Macrocyclic 18-Crown-6 Polyether Additives on Catalysis by Bicyclic Nickel Complexes

AUTHOR(S): Matienko, L. I.; Mosolova, L. A.
CORPORATE SOURCE: Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2003), 44(2), 221-228
CODEN: KICAA8; ISSN: 0023-1584
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133158

AB The catalytic activity of the two-component catalytic system based on nickel bis(enaminoacetonate) (enamac) and 18-crown-6 (18C6) macrocyclic polyether is studied in ethylbenzene oxidation by mol. oxygen. The {Ni(enamac)2 & 18-crown-6} system is a more active catalyst of ethylbenzene oxidation into α-phenylethyl hydroperoxide compared to Ni(enamac)2 and the {Ni(acac)2 & 18-crown-6} system. The formation of Ni(enamac)2-18-crown-6 complex is confirmed both kinetically and spectroscopically. It is suggested that a rise in the oxidation selectivity is due to Ni(enamac)2 transformation activated by 18-crown-6. The order of oxidation product formation at different oxidation stages is determined The activity of catalysts in the elementary steps of the chain process is discussed.

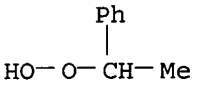
IT **15170-64-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(effect of macrocyclic crown polyether additives on **catalysis** by bicyclic nickel complexes)
RN 15170-64-6 CAPLUS
CN Nickel, bis[4-(imino-κN)-2-pentanonato-κO]- (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RGT (Reagent)**; **RACT (Reactant or reagent)**
(effect of macrocyclic crown polyether additives on catalysis by bicyclic nickel complexes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **3071-32-7P**, α-Phenylethyl hydroperoxide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(effect of macrocyclic crown polyether additives on catalysis by

bicyclic nickel complexes)
RN 3071-32-7 CAPLUS
CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 43 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:450363 CAPLUS
DOCUMENT NUMBER: 137:33200
TITLE: Preparation of oxiranes by the epoxidation of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides
INVENTOR(S): Vaporciyan, Garo Garbis; Murray, Brendan Dermot
PATENT ASSIGNEE(S): Shell Oil Company, Neth.
SOURCE: U.S. Pat. Appl. Publ., 4 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002072622	A1	20020613	US 2000-736522	20001213
US 6455712	B2	20020924		
WO 2002048125	A2	20020620	WO 2001-EP14748	20011213
WO 2002048125	A3	20030410		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
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WO 2002048126	A2	20020620	WO 2001-EP14750	20011213
WO 2002048126	A3	20030417		
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WO 2002048127	A2	20020620	WO 2001-EP14751	20011213
WO 2002048127	A3	20030424		

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AU 2002016112	A5	20020624	AU 2002-16112	20011213
AU 2002017114	A5	20020624	AU 2002-17114	20011213
AU 2002038433	A5	20020624	AU 2002-38433	20011213
EP 1343776	A2	20030917	EP 2001-986878	20011213
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EP 1347962	A2	20031001	EP 2001-270532	20011213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EP 1366031	A2	20031203	EP 2001-270533	20011213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001016099	A	20031223	BR 2001-16099	20011213
BR 2001016100	A	20031223	BR 2001-16100	20011213
BR 2001016101	A	20031223	BR 2001-16101	20011213
JP 2004517841	T2	20040617	JP 2002-549656	20011213
JP 2004517842	T2	20040617	JP 2002-549657	20011213
TW 593298	B	20040621	TW 2001-90130928	20011213
JP 2004525870	T2	20040826	JP 2002-549658	20011213
PRIORITY APPLN. INFO.:			US 2000-736522 A	20001213
			WO 2001-EP14748 W	20011213
			WO 2001-EP14750 W	20011213
			WO 2001-EP14751 W	20011213

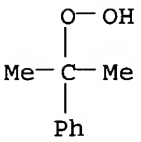
OTHER SOURCE(S): CASREACT 137:33200

AB A process for preparing epoxides, which process comprises: (i) oxidizing an alkylaryl (e.g., cumene) to obtain a stream comprising alkylaryl hydroperoxide (e.g., cumene hydroperoxide); (ii) contacting at least a part of the alkylaryl hydroperoxide obtained in step (i) with an olefin (e.g., 1-octene) in the presence of a catalyst (e.g., Ti/SiO2) to obtain a product stream comprising an oxirane compound (e.g., n-hexyloxirane) and an alkylaryl hydroxyl compound (e.g., 2-phenyl-2-propanol); (iii) optionally reacting part of the alkylaryl hydroperoxide obtained in step (i) to obtain a mixture comprising (a) phenol, and (b) a ketone and/or aldehyde,and (c) optionally byproducts; (iv) separating the oxirane compound from the product stream of step (ii) to obtain (a) a residual product stream and (b) oxirane, and (v) contacting at least a part of the residual product stream with hydrogen (i.e., hydrogenolysis) to obtain the alkylaryl compound, wherein at least a part of said alkylaryl is recycled to step (i).

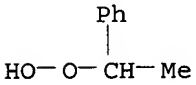
IT **80-15-9P**, Cumene hydroperoxide **3071-32-7P**, Ethylbenzene hydroperoxide
RL: **IMF (Industrial manufacture)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(epoxidizing agent; preparation of oxiranes by the epoxidn. of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides)

RN 80-15-9 CAPLUS

CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



RN 3071-32-7 CAPLUS
CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



IT **7440-50-8**, Copper, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(hydrogenolysis **catalysts** in a preparation of oxiranes by the epoxidn. of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides using)
RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of oxiranes by the epoxidn. of alkenes with aralkyl hydroperoxides and regeneration of the hydroperoxides)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

L34 ANSWER 44 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:672190 CAPLUS
DOCUMENT NUMBER: 137:203018
TITLE: Process for oxidation of organic substrates
INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002249451	A2	20020906	JP 2001-46389	20010222

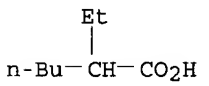
PRIORITY APPLN. INFO.: JP 2001-46389 20010222

AB The title process comprises contacting an organic substrate with oxygen in the presence of N-hydroxy cyclic imide, ≤ 0.1 mol% cobalt compound (relative to substrate), and ≤ 0.1 mol% vanadium compound (relative to substrate). Cyclohexane was oxidized by the title process to give cyclohexanone, cyclohexanol, cyclohexyl hydroperoxide, and adipic acid in 7.6%, 0.06%, 2.5%, and 1.3% yields, resp.

IT **136-52-7**, Cobalt octoate
RL: **CAT (Catalyst use)**; USES (Uses)
(process for oxidation of organic substrates)

RN 136-52-7 CAPLUS

CN Hexanoic acid, 2-ethyl-, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

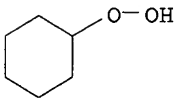


●1/2 Co(II)

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process for oxidation of organic substrates)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for oxidation of organic substrates in presence of cobalt octanoate and vanadium naphthenate as catalysts)

RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 45 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:672188 CAPLUS

DOCUMENT NUMBER: 137:201098

TITLE: Continuous oxidation of organic substrates with

molecular oxygen and with high efficiency, and manufacture of oxygen-containing compounds by the method
INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002249450	A2	20020906	JP 2001-44752	20010221
PRIORITY APPLN. INFO.:			JP 2001-44752	20010221

OTHER SOURCE(S): CASREACT 137:201098

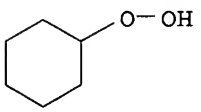
AB Organic substrates are continuously oxidized with supplying mixts. of the substrates, N-hydroxylated cyclic imides, and O-containing gas to solns. containing the imides whose concentration is higher than that of the imides in the supplying mixts. Thus, air, a mixture of cyclohexane (I) and Co octylate (II), and a mixture of I, 0.25 weight% N-hydroxyphthalimide (III), and cyclohexanol (IV) were continuously supplied to a mixture of I, 0.5 weight% III, II, and IV over 5 h with retention time 1 h to give 0.5% adipic acid, and cyclohexanone, IV, and cyclohexyl hydroperoxide with 3.5% combined yield.

IT **6700-85-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(continuous oxidation of organic substrates with mol. oxygen in presence of transition metal **catalysts** and N-hydroxylated cyclic imides)
RN 6700-85-2 CAPLUS
CN Octanoic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)

$HO_2C-(CH_2)_6-Me$

●x Co(x)

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**
(continuous oxidation of organic substrates with mol. oxygen in presence of transition metal catalysts and N-hydroxylated cyclic imides)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)

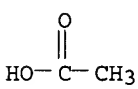


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(continuous oxidation of organic substrates with mol. oxygen in presence of transition metal catalysts and N-hydroxylated cyclic imides)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

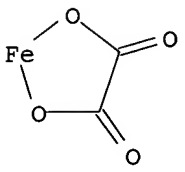
L34 ANSWER 46 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:514248 CAPLUS
DOCUMENT NUMBER: 137:63038
TITLE: Oxidation of organic compounds without decompositions of imides
INVENTOR(S): Tani, Nobuhiro; Murata, Shuzo
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Daicel Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002193855	A2	20020710	JP 2000-395772	20001226
PRIORITY APPLN. INFO.:			JP 2000-395772	20001226

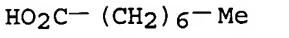
OTHER SOURCE(S): CASREACT 137:63038
AB Organic substrates are oxidized by O in the presence of N-hydroxy cyclic imides and ≤0.1 mol% (to substrates) ≥2 transition metal compds. chosen from Co, Ce, Ti, Fe, and Cu compds. Cyclohexane was oxidized by O-containing gas in MeCN in the presence of N-hydroxyphthalimide, 0.000093 mol Co(II) octylate, and 0.000099 mol Ti(OPr-i)4 at 100° under 0.9 MPa for 2.6 h to give cyclohexanone, cyclohexanol, cyclohexyl hydroperoxide, and adipic acid with 47, 8, 25, and 9% selectivity, resp. Remaining of N-hydroxyphthalimide was 73%.
IT **142-71-2**, Copper(II) acetate **516-03-0**, Iron(II) oxalate **1588-79-0** **21679-46-9**, Cobalt(III) acetylacetonate
RL: **CAT (Catalyst use)**; USES (Uses)
(decomposition inhibitor; oxidation of organic compds. without decompns. of imides)
RN 142-71-2 CAPLUS
CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)



RN 516-03-0 CAPLUS
CN Iron, [ethanedioato(2-)-κO1,κO2]- (9CI) (CA INDEX NAME)

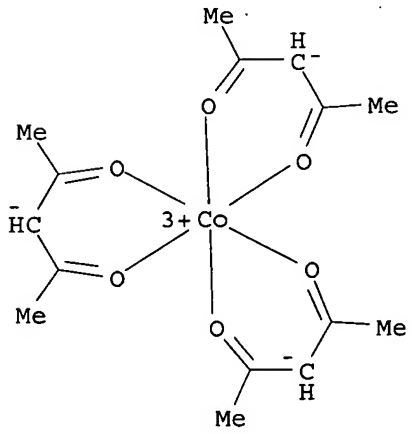


RN 1588-79-0 CAPLUS
CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

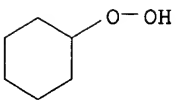


●1/2 Co(II)

RN 21679-46-9 CAPLUS
CN Cobalt, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(oxidation of organic compds. without decompns. of imides)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)

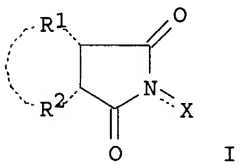


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of organic compds. without decompns. of imides)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 47 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:235931 CAPLUS
DOCUMENT NUMBER: 136:294727
TITLE: Method for preparing organic compounds using imides and nitric acids
INVENTOR(S): Ishii, Yasutaka; Tatsumi, Atsuo; Nakano, Tatsuya
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002088077	A2	20020327	JP 2001-111912	20010410
PRIORITY APPLN. INFO.:			JP 2000-209205 A	20000711

OTHER SOURCE(S): CASREACT 136:294727; MARPAT 136:294727
GI

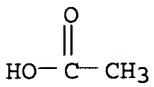


I

AB Disclosed is a highly selective method with high recovery rate for producing organic compds. by addition reaction and/or substitution reaction under gentle conditions. The addition and/or substitution reaction products are prepared by reacting radical forming compound with radical capturing compound in the presence of imide (I; R1 = alkyl; R2= aryl, or R1/R2 = aromatic or non-aromatic ring, and X = O or OH) and nitric acid or nitrous acid salt.

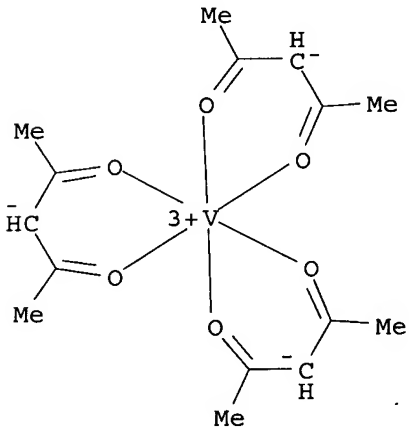
IT **7782-44-7**, Oxygen, reactions
RL: **RGT (Reagent)**; **RACT (Reactant or reagent)**
(gas containing; preparation of organic compds. by reacting radical-forming agent
with radical-capturing agent in the presence of imide and nitric or nitrous acid)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **71-48-7**, Cobalt acetate **13476-99-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of organic compds. by reacting radical-forming agent with radical-capturing agent in the presence of imide and nitric or nitrous acid)
RN 71-48-7 CAPLUS
CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



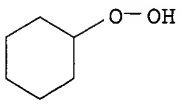
●1/2 Co(II)

RN 13476-99-8 CAPLUS
CN Vanadium, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of organic compds. by reacting radical-forming agent with

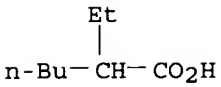
radical-capturing agent in the presence of imide and nitric or nitrous acid)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



L34 ANSWER 48 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:405758 CAPLUS
DOCUMENT NUMBER: 136:401466
TITLE: Oxidative process and catalyst system for preparing cyclohexanone, cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas
INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro
PATENT ASSIGNEE(S): Sumitomo Chemical Company Limited, Japan; Daicel Chemical Industries, Ltd.
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

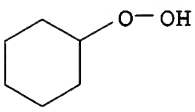
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1209143	A1	20020529	EP 2001-127410	20011123
EP 1209143	B1	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002161056	A2	20020604	JP 2000-357363	20001124
US 2002065436	A1	20020530	US 2001-992012	20011126
US 6459002	B2	20021001		

PRIORITY APPLN. INFO.: JP 2000-357363 A 20001124
OTHER SOURCE(S): CASREACT 136:401466
AB Cyclohexanone, cyclohexanol and/or cyclohexyl hydroperoxide are prepared at a high productivity by the oxidation of cyclohexane with an oxygen-containing gas using a catalyst system comprising a cyclic N-hydroxyimide (e.g., N-hydroxyphthalimide) and a transition metal compound (e.g., cobalt octoate) in the presence of cyclohexanone, and optional cyclohexanol, which is/are added to the reaction system while conducting the oxidation
IT **136-52-7**, Cobalt octoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidative **catalyst** system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)
RN 136-52-7 CAPLUS
CN Hexanoic acid, 2-ethyl-, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(oxidative process and catalyst system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidative process and catalyst system for preparing cyclohexanone and cyclohexanol and cyclohexyl hydroperoxide from cyclohexane in the presence of an oxygen-containing gas)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

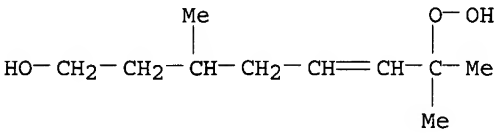
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 49 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:386166 CAPLUS
DOCUMENT NUMBER: 137:201007
TITLE: "Dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions
AUTHOR(S): Nardello, Veronique; Herve, Melanie; Alsters, Paul L.; Aubry, Jean-Marie
CORPORATE SOURCE: LCOM, Equipe de Recherches "Oxydation et Formulation", ESA CNRS 8009, ENSCL, Villeneuve d'Ascq, 59652, Fr.
SOURCE: Advanced Synthesis & Catalysis (2002), 344(2), 184-191
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201007
AB The molybdate-catalyzed "dark" singlet oxygenation of hydrophobic compds.

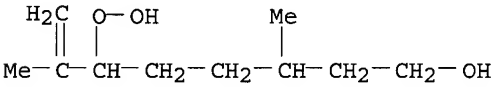
with hydrogen peroxide proceeds efficiently with low catalyst loadings (10-3 mol%) in chlorine-free w/o microemulsions. These micro-heterogeneous systems are composed of sodium dodecyl sulfate (SDS)/n-butanol/water/organic phase, the latter being either a "green" solvent such as Et acetate or a liquid substrate, such as α-terpinene or β-citronellol. Very high reactor yields with improved product/SDS ratio can be obtained for the "dark" singlet oxygenation of such liquid substrates.

IT **81113-73-7P 81113-74-8P**
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
("dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)

RN 81113-73-7 CAPLUS
CN 5-Octen-1-ol, 7-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)

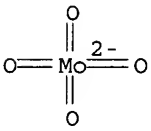


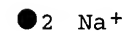
RN 81113-74-8 CAPLUS
CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



IT **7631-95-0**, Sodium molybdate (Na2MoO4)
RL: **CAT (Catalyst use)**; USES (Uses)
(disproportionation **catalyst**; "dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)

RN 7631-95-0 CAPLUS
CN Molybdate (MoO42-), disodium, (T-4)- (9CI) (CA INDEX NAME)





IT **7782-44-7**, Oxygen, reactions
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); **RCT (Reactant)**; FORM (Formation, nonpreparative); PROC

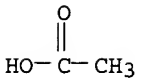
(Process); **RACT (Reactant or reagent)**
(singlet; "dark" singlet oxygenation of hydrophobic substrates in environmentally friendly microemulsions)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 50 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:450919 CAPLUS
DOCUMENT NUMBER: 135:33339
TITLE: Process and catalysts for preparing a ketone, an alcohol and a hydroperoxide by the oxidation of a hydrocarbon
INVENTOR(S): Murata, Shuzo; Tani, Nobuhiro; Asano, Hiroyuki
PATENT ASSIGNEE(S): Sumitomo Chemical Company Limited, Japan; Daicel Chemical Industries, Ltd.
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

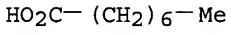
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1108701	A1	20010620	EP 2000-311105	20001213
EP 1108701	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001233809	A2	20010828	JP 2000-343302	20001110
ES 2197852	T3	20040116	ES 2000-311105	20001213
CN 1302788	A	20010711	CN 2000-137320	20001214
US 2001016670	A1	20010823	US 2000-735926	20001214
US 6479705	B2	20021112		

PRIORITY APPLN. INFO.: JP 1999-354216 A 19991214
OTHER SOURCE(S): CASREACT 135:33339
AB A process for preparing a ketone (e.g., cyclohexanone), an alc. (e.g., cyclohexanol), and/or a hydroperoxide (e.g., cyclohexyl hydroperoxide) in high yield and selectivity comprises reacting a hydrocarbon (e.g., cyclohexane) with mol. oxygen in the presence of a cyclic N-hydroxyimide (e.g., N-hydroxyphthalimide) and a transition metal compound catalyst (e.g., cobalt diacetate) system, where the oxygen-containing gas is supplied to the reaction system and at the same time a gas containing 1-10% (by volume) of oxygen is discharged from the reaction system.
IT **71-48-7**, Cobalt diacetate **1588-79-0**, Cobalt dioctanoate **14284-89-0**, ManganeseIII acetylacetonate
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts** for preparing a ketone and an alc. and a hydroperoxide by the oxidation of a hydrocarbon)
RN 71-48-7 CAPLUS
CN Acetic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



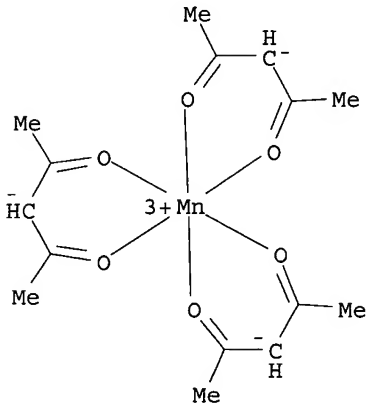
●1/2 Co(II)

RN 1588-79-0 CAPLUS
CN Octanoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)

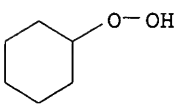


●1/2 Co(II)

RN 14284-89-0 CAPLUS
CN Manganese, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI)
(CA INDEX NAME)



IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(process and catalysts for preparing a ketone and an alc. and a hydroperoxide by the oxidation of a hydrocarbon)
RN 766-07-4 CAPLUS
CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process and catalysts for preparing a ketone and an alc. and a hydroperoxide by the oxidation of a hydrocarbon)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

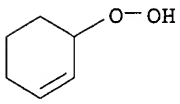
L34 ANSWER 51 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:883290 CAPLUS
DOCUMENT NUMBER: 136:216383
TITLE: Dioxygen affinity and catalytic performance of bis-(furaldehyde) Schiff bases Co(II) complexes in cyclohexene oxidation
AUTHOR(S): Sun, Bin; Chen, Jun Ru; Hu, Jia Yuan; Li, Xian Jun
CORPORATE SOURCE: Department of Chemistry, Sichuan University, Chengdu, 610064, Peop. Rep. China
SOURCE: Chinese Chemical Letters (2001), 12(11), 1043-1046
CODEN: CCLEE7; ISSN: 1001-8417
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:216383
AB Oxygenation consts. and thermodn. parameters ΔH° and ΔS° of Co (II) complexes with three bis(furaldehyde) Schiff bases (1, 2, 3, 4) were obtained by measuring saturated dioxygen uptake of these complexes in pyridine at different temperature These complexes could activate mol. O and were used as catalysts in cyclohexene oxidation The influence of ligand structure on the dioxygen affinity and catalytic activity of the complexes were discussed.
IT **7782-44-7**, Oxygen, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(carrier mimic for; dioxygen affinity and catalytic performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **7646-79-9**, Cobaltous chloride, reactions
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(**catalyst** precursor; dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)
RN 7646-79-9 CAPLUS

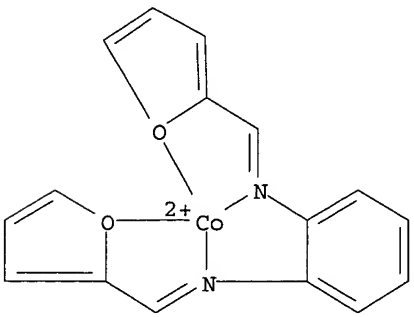
CN Cobalt chloride (CoCl2) (8CI, 9CI) (CA INDEX NAME)

Cl—Co—Cl

IT **4845-05-0P**
RL: **BYP (Byproduct)**; **PREP (Preparation)**
(dioxygen affinity and catalytic performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)
RN 4845-05-0 CAPLUS
CN Hydroperoxide, 2-cyclohexen-1-yl (9CI) (CA INDEX NAME)

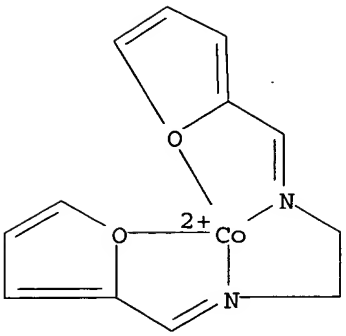


IT **402594-30-3 402594-31-4 402594-32-5**
402594-33-6
RL: **CAT (Catalyst use)**; CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)
RN 402594-30-3 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



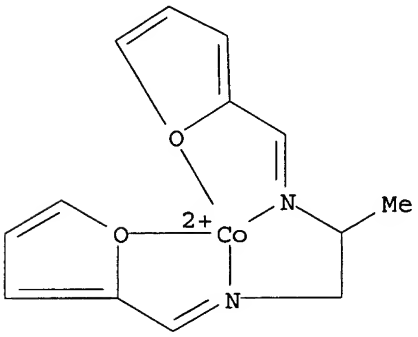
●2 Cl⁻

RN 402594-31-4 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-ethanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



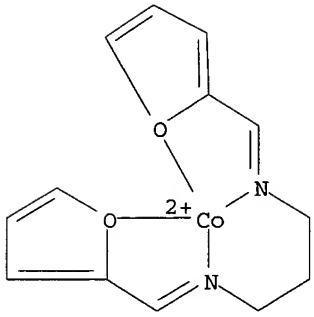
●2 Cl⁻

RN 402594-32-5 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-propanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



●2 Cl⁻

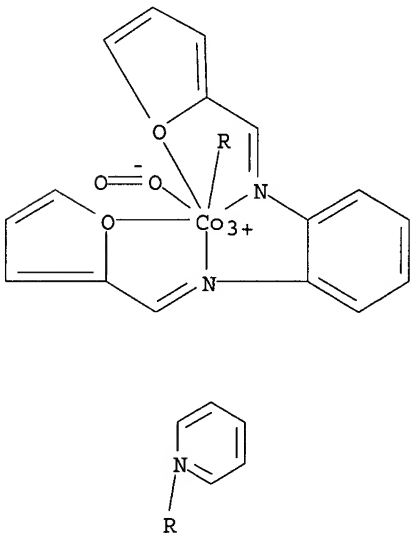
RN 402594-33-6 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,3-propanediamine-κN,κN']-, dichloride (9CI) (CA INDEX NAME)



●2 Cl⁻

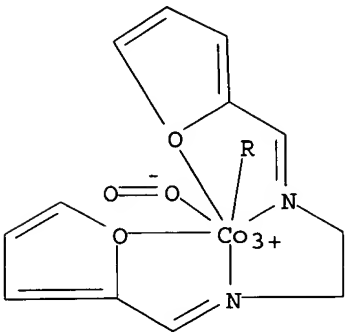
IT **402594-38-1 402594-39-2 402594-40-5**
402594-41-6
RL: **CAT (Catalyst use)**; CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(oxygen carrier; dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

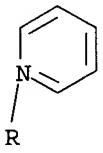
RN 402594-38-1 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN'](pyridine)superoxido-, (OC-6-43)- (9CI) (CA INDEX NAME)



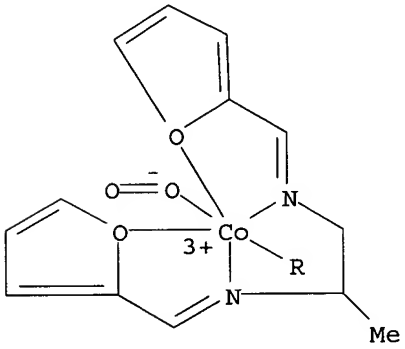
RN 402594-39-2 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-ethanediamine-

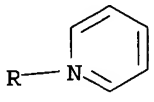
κN,κN'](pyridine)superoxido-, (OC-6-43)- (9CI) (CA INDEX NAME)



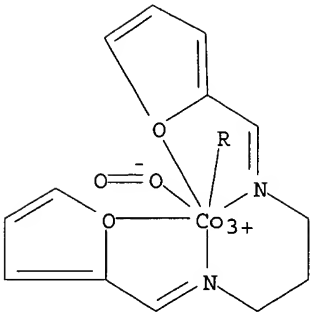


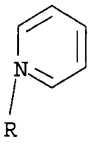
RN 402594-40-5 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-propanediamine-κN,κN'](pyridine)superoxido-, (OC-6-65)- (9CI) (CA INDEX NAME)





RN 402594-41-6 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,3-propanediamine-κN,κN'](pyridine)superoxido-, (OC-6-43)- (9CI) (CA INDEX NAME)

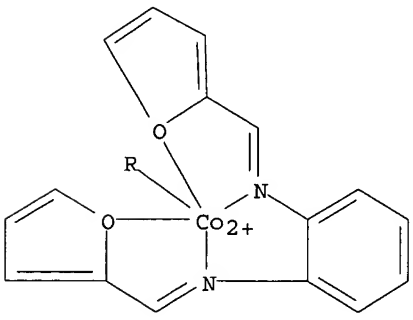


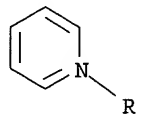


IT **402594-34-7 402594-35-8 402594-36-9**
402594-37-0
RL: **CAT (Catalyst use)**; CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(oxygenation of **precatalyst**; dioxygen affinity and **catalytic** performance of bis(furaldehyde) Schiff base Co(II) complexes in cyclohexene oxidation)

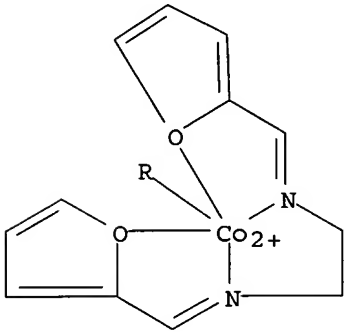
RN 402594-34-7 CAPLUS

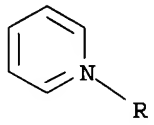
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-benzenediamine-κN,κN'](pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)



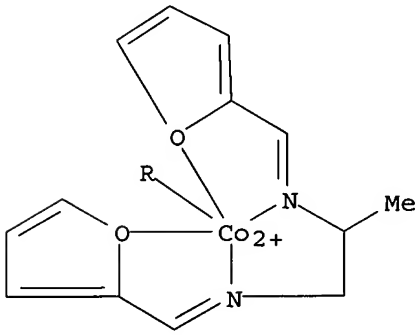


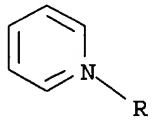
RN 402594-35-8 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-ethanediamine-κN,κN'](pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)



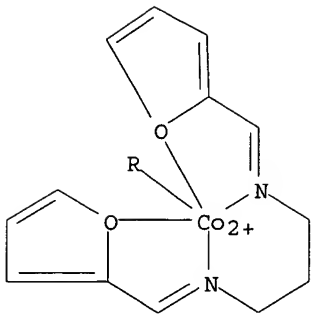


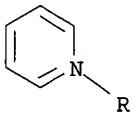
RN 402594-36-9 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,2-propanediamine-κN,κN'](pyridine)-, (SP-5-54)- (9CI) (CA INDEX NAME)





RN 402594-37-0 CAPLUS
CN Cobalt(2+), [N,N'-bis[(2-furanyl-κO)methylene]-1,3-propanediamine-κN,κN'](pyridine)-, (SP-5-32)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 52 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:742044 CAPLUS
DOCUMENT NUMBER: 133:281926
TITLE: Singlet oxygen oxidation of organic substrates
INVENTOR(S): Aubry, Jean-Marie; Rataj-Nardello, Veronique; Alsters, Paul
PATENT ASSIGNEE(S): DSM Fine Chemicals Austria G.m.b.H., Austria
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061524	A1	20001019	WO 2000-EP2552	20000323
W: AE, AL, AM, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AT 9900647	A	20010515	AT 1999-647	19990413
AT 408546	B	20011227		
CA 2369589	AA	20001019	CA 2000-2369589	20000323
EP 1169281	A1	20020109	EP 2000-922539	20000323
EP 1169281	B1	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002541227	T2	20021203	JP 2000-610802	20000323
AT 259764	E	20040315	AT 2000-922539	20000323

PT 1169281	T	20040531	PT 2000-922539		20000323
ES 2211533	T3	20040716	ES 2000-922539		20000323
PRIORITY APPLN. INFO.:			AT 1999-647	A	19990413
			WO 2000-EP2552	W	20000323

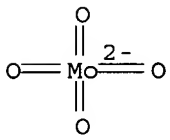
OTHER SOURCE(S): CASREACT 133:281926

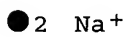
AB The invention relates to a method for oxidizing organic substrates using 1O2 in which hydrophobic organic substrates that react with 1O2 are added to an organic solvent in the presence of a heterogeneous or homogeneous catalyst with 30-70% being comprised of H2O2. Afterwards, H2O2 is catalytically decomposed into water and 1O2, and the oxidation into corresponding oxidation products ensues. Thus, α-terpinene is added to methanol containing Na2MoO4·2H2O followed by 45 μl H2O2 to give 100% ascaridol.

IT **7631-95-0**, Sodium molybdate
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous **catalyst**)

RN 7631-95-0 CAPLUS

CN Molybdate (MoO42-), disodium, (T-4)- (9CI) (CA INDEX NAME)





IT **7782-44-7D**, Oxygen, singlet, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous catalyst)

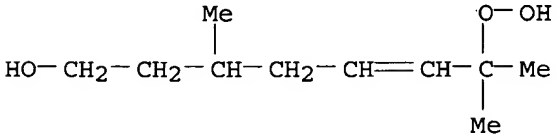
RN 7782-44-7 CAPLUS

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

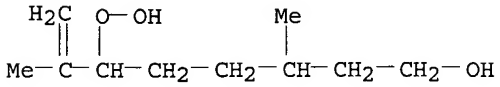
IT **81113-73-7P 81113-74-8P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(oxidation of organic substrates with singlet oxygen in the presence of a heterogeneous or homogeneous catalyst)

RN 81113-73-7 CAPLUS

CN 5-Octen-1-ol, 7-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)



RN 81113-74-8 CAPLUS
CN 7-Octen-1-ol, 6-hydroperoxy-3,7-dimethyl- (9CI) (CA INDEX NAME)

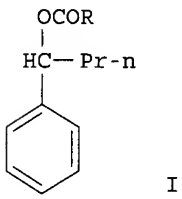


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 53 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:12136 CAPLUS
DOCUMENT NUMBER: 142:56002
TITLE: An improved process for the preparation of phenylpropylcarbinyl esters of organic acids
INVENTOR(S): Shende, Bansidhar Wasudeo; Shah, Naresh Fulchand; Chaudhuri, Basab
PATENT ASSIGNEE(S): Herdillia Chemicals Ltd., India
SOURCE: Indian, 16 pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 185059	A	20001028	IN 1996-BO103	19960222

PRIORITY APPLN. INFO.: IN 1996-BO103 19960222
OTHER SOURCE(S): CASREACT 142:56002; MARPAT 142:56002
GI



I

AB An improved process for the preparation of phenylpropylcarbinyl esters of the formula I wherein R represents an alkyl group is reported. The process involved oxidation of n-butylbenzene with oxygen or a gas containing it, at a temperature in the range of 120 to 140°C, pH in the range of 5.5 to 6.5, maintaining the content of water in the reaction mixture in the range of 2 to 8% weight/weight, pressure in the range of 2 to 10 kg/cm2 and the space velocity of the oxygen-containing gas in the range of 1 to 4 cm/s, gave a mixture containing unreacted n-butylbenzene, 1-phenylbutyl hydroperoxide 1-phenyl-1-butanone and phenylpropylcarbinol. Further, conversion of 1-phenylbutyl hydroperoxide from the above mixture to phenylpropylcarbinol by direct hydrogenation with hydrogen at a temperature in the range of 30 to

70°C and pressure in the range of 3 to 10 kg/cm2 in the presence of a hydrogenation catalyst gave a mixture containing n-butylbenzene and 1-phenyl-1-butanone. The reduction of 1-phenyl-1-butanone in the mixture obtained from the previous step by hydrogenation at a temperature in the range of 80 to 180°C and a pressure in the range of 5-75 kg/cm2 in the presence of a hydrogenation catalyst resulted in a new mixture containing n-butylbenzene and phenylpropylcarbinol. Finally, phenylpropylcarbinol was separated from the mixture by fractional distillation, which upon acylation yielded the title compds.

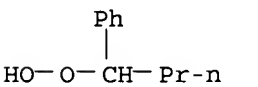
IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalyst** hydrogenation; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)
RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O═O

IT **58687-89-1P**
RL: **IMF (Industrial manufacture)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by hydrogenation of phenylbutyl hydroperoxide and phenylbutanone intermediates)
RN 58687-89-1 CAPLUS
CN Hydroperoxide, 1-phenylbutyl (9CI) (CA INDEX NAME)

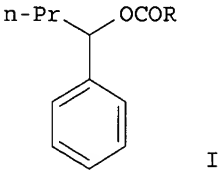


L34 ANSWER 54 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:55319 CAPLUS
DOCUMENT NUMBER: 142:93537

TITLE: An improved process for the preparation of phenylpropylcarbinyl esters of organic acids
INVENTOR(S): Shende, Bansidhar Wasudeo; Shah, Naresh Fulchand; Chaudhuri, Basab
PATENT ASSIGNEE(S): Herdillia Chemicals Ltd., India
SOURCE: Indian, 14 pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 185058	A	20001028	IN 1996-BO102	19960222
PRIORITY APPLN. INFO.:			IN 1996-BO102	19960222

OTHER SOURCE(S): CASREACT 142:93537; MARPAT 142:93537
GI



I

AB An improved process for the preparation of phenylpropylcarbinyl esters I (R = alkyl group) from n-butylbenzene which comprises, oxidation of n-butylbenzene by oxygen of a gas containing it under specified condition resulted in a mixture containing unreacted n-butylbenzene, 1-phenylbutyl hydroperoxide, 1-phenyl-1-butanone and phenylpropylcarbinol. Addition of cyclic olefin to above mixture obtained from previous step at a temperature in the range of 60 to 110°C under autogenous pressure in the presence of an epoxidn. catalyst resulted in conversion of 1-phenylbutyl hydroperoxide present in the mixture to phenylpropylcarbinol and the cyclic olefin to its epoxide, separating the unconverted cyclic olefin and its epoxide by fractional distillation was done to obtain the appropriate epoxide as a co-product. Reduction of 1-phenyl-1-butanone in the mixture obtained from the above step via hydrogenation at a temperature in the range of 80 to 180°C and a pressure in the range of 5-75 kg/cm2 in the presence of a hydrogenation catalyst yielded a mixture containing n-butylbenzene and phenylpropylcarbinol. Separation of phenylpropylcarbinol from the mixture was achieved by fractional distillation Finally, acylation of phenylpropylcarbinol by conventional methods afforded the phenylpropylcarbinyl esters I.

IT **7440-02-0**, Raney nickel, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts** hydrogenation; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent hydrogenation)

RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

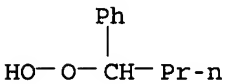
Ni

IT **30568-96-8**, Molybdenum stearate
RL: **CAT (Catalyst use)**; USES (Uses)
(epoxidn. **catalyst**; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent hydrogenation)
RN 30568-96-8 CAPLUS
CN Octadecanoic acid, molybdenum salt (9CI) (CA INDEX NAME)

$HO_2C-(CH_2)_{16}-Me$

●x Mo(x)

IT **58687-89-1P**
RL: **IMF (Industrial manufacture)**; RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent hydrogenation)
RN 58687-89-1 CAPLUS
CN Hydroperoxide, 1-phenylbutyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidizing agent; industrial preparation of phenylpropylcarbinyl esters from phenylpropylcarbinol via oxidation of butylbenzene followed by epoxidn. of cyclohexene by phenylbutyl hydroperoxide intermediate and subsequent hydrogenation)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

L34 ANSWER 55 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:426679 CAPLUS
DOCUMENT NUMBER: 133:266543
TITLE: The oxidation of ethylbenzene and other alkylaromatics by dioxygen catalyzed by iron(III) tetrakis(pentafluorophenyl)porphyrin and related iron porphyrins
AUTHOR(S): Evans, Steven; Lindsay Smith, John R.
CORPORATE SOURCE: Department of Chemistry, University of York, York, YO10 5DD, UK
SOURCE: Perkin 2 (2000), (7), 1541-1552
CODEN: PRKTFO
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:266543

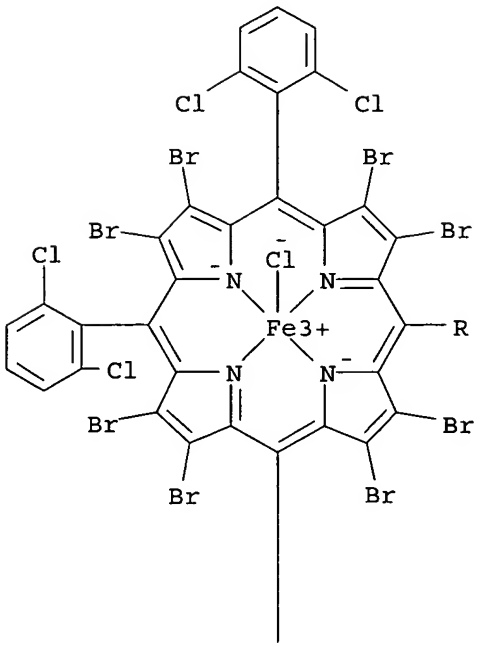
AB The oxidation of ethylbenzene with dioxygen catalyzed by iron(III) porphyrins in a solvent free system was studied over the temperature range 30-110 °C. The time dependence of the formation of the three main products, 1-phenylethanol, acetophenone and 1-phenylethyl hydroperoxide, and the fate of the iron porphyrin are interpreted in terms of a free radical autoxidn. mechanism. The yields of the oxidation products are determined by the rate of reaction and by the lifetime of the catalyst. Catalyst degradation is shown to involve reaction of the porphyrin ligand with 1-phenylethoxyl and 1-phenylethylperoxyl radicals. The disadvantages of increased induction periods and longer reaction times of the oxidns. observed at lower reaction temps. are counter balanced by increased catalyst turnovers. Less extensive studies on the oxidns. of toluene, cumene, (2-methylpropyl)benzene and tert-butylbenzene support the overall mechanism proposed for ethylbenzene. A comparative study using the catalysts iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin and iron(III) tetrakis(pentafluorophenyl)porphyrin and five of its derivs. reveals that halogenation of the β-pyrrole positions markedly increases the activity of the catalysts but not the stability of the porphyrin towards degradation The highest yields were obtained with the μ-oxo dimer of iron(III) tetrakis(pentafluorophenyl)porphyrin and iron(III) tetrakis(4-dimethylamino-2,3,5,6-tetrafluorophenyl)porphyrin.

IT **81245-20-7**, μ-Oxobis[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato]diiron **107053-17-8**, Chloro[octabromotetrakis(2,6-dichlorophenyl)porphyrinato]iron
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation of (alkyl)benzenes by dioxygen **catalyzed** by iron porphyrins)

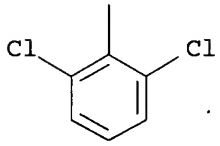
RN 81245-20-7 CAPLUS
CN Iron, μ-oxobis[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]di- (9CI) (CA INDEX NAME)

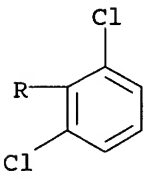
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 107053-17-8 CAPLUS
CN Iron, chloro[2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

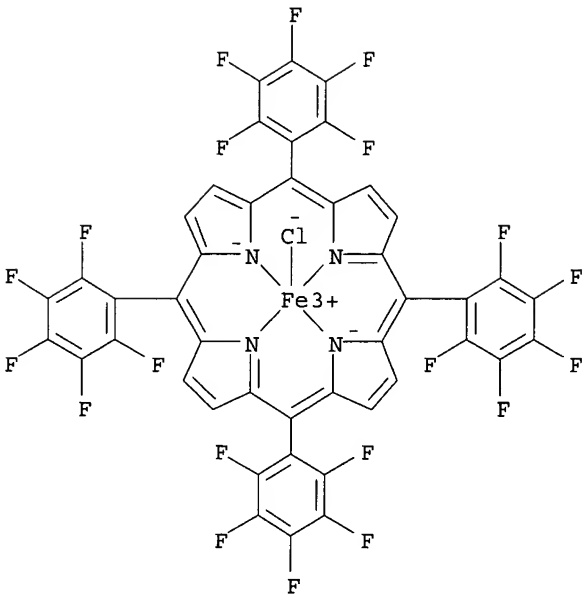




IT **36965-71-6P**, Chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinatoiron(III)
RL: **CAT (Catalyst use)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(oxidation of (alkyl)benzenes by dioxygen **catalyzed** by iron porphyrins)

RN 36965-71-6 CAPLUS

CN Iron, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

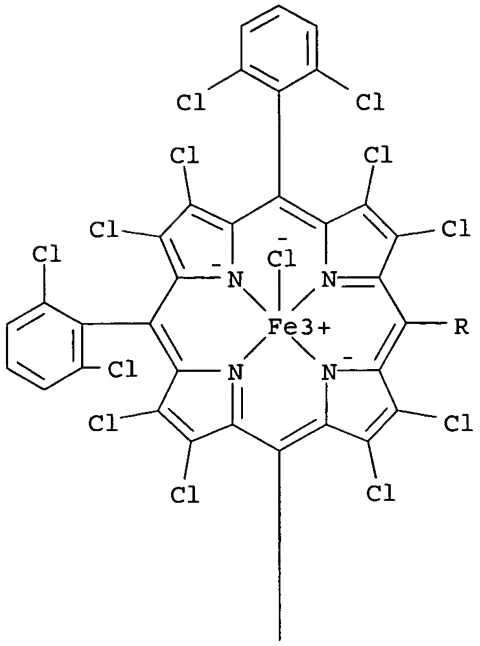


IT **120676-09-7P**, Chloro[octachlorotetrakis(2,6-dichlorophenyl)porphyrinato]iron **131917-66-3P** **134131-11-6P**, Iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin **177532-06-8P**, Chloro[5,10,15,20-tetrakis(tetrafluoro4-phenoxyphenyl)-21H,23H-porphinatoiron(III)
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(oxidation of (alkyl)benzenes by dioxygen **catalyzed** by iron porphyrins)

RN 120676-09-7 CAPLUS

CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

PAGE 1-A



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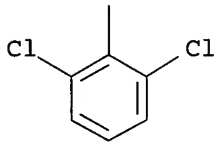
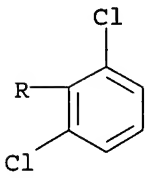
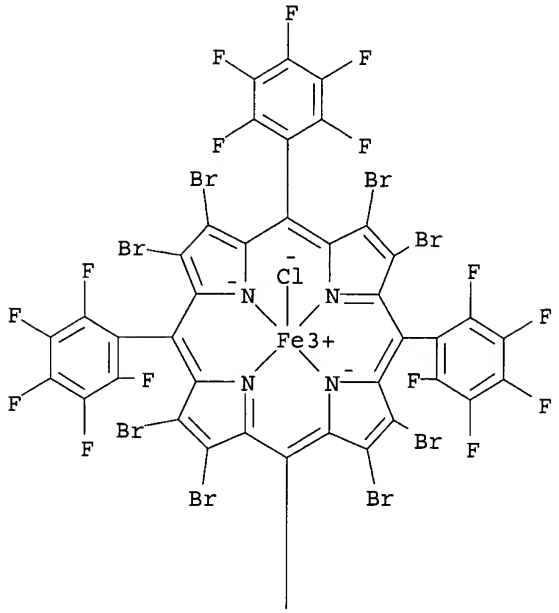




RN 131917-66-3 CAPLUS
CN Iron, chloro[2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

PAGE 1-A



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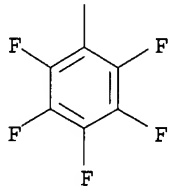
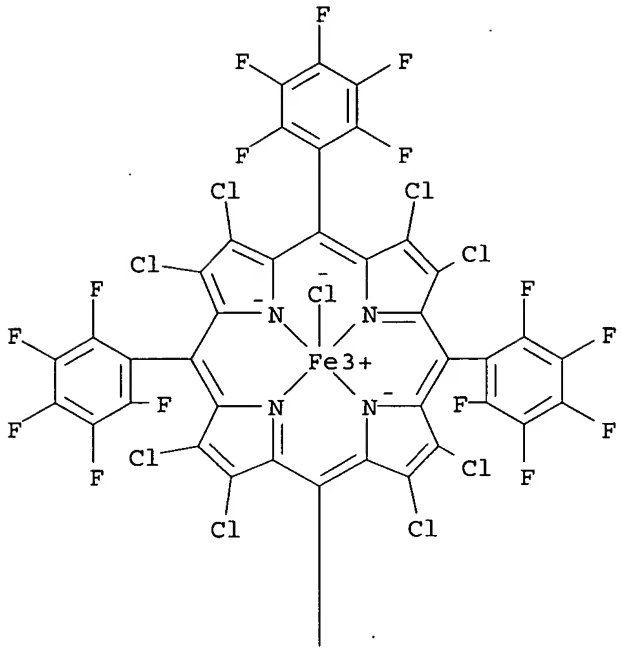


RN 134131-11-6 CAPLUS
CN Iron, chloro[2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

PAGE 1-A



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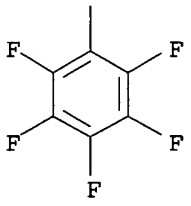
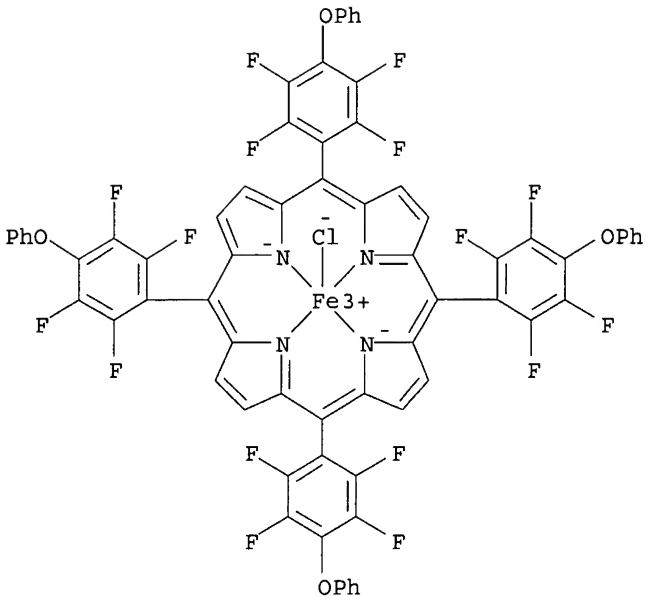
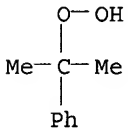


RN 177532-06-8 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(2,3,5,6-tetrafluoro-4-phenoxyphenyl)-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

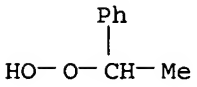


IT **7782-44-7**, Dioxygen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(oxidation of (alkyl)benzenes by dioxygen catalyzed by iron porphyrins)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **80-15-9P**, Cumene hydroperoxide
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(oxidation of cumene by dioxygen catalyzed by iron porphyrins)
RN 80-15-9 CAPLUS
CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

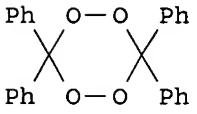


IT **3071-32-7P**, 1-Phenylethyl hydroperoxide
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(oxidation of ethylbenzene by dioxygen catalyzed by iron porphyrins)
RN 3071-32-7 CAPLUS
CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 56 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:296195 CAPLUS
DOCUMENT NUMBER: 133:43120
TITLE: Ozonation of 1,1,2,2-tetraphenylethene revisited: evidence for electron-transfer oxygenations
AUTHOR(S): Schank, Kurt; Beck, Horst; Buschlinger, Michael; Eder, Jorg; Heisel, Thomas; Pistorius, Susanne; Wagner, Christiane
CORPORATE SOURCE: Department of Organic Chemistry, University of Saarland, Saarbrucken, D-66041, Germany
SOURCE: Helvetica Chimica Acta (2000), 83(4), 801-826
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
GI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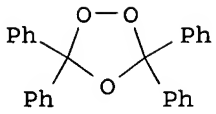
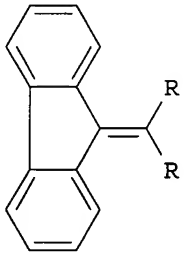
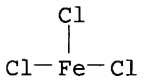

II


III

AB Ozonolysis of 1,1,2,2-tetraphenylethene (TPE, 1) were described many times in the literature, but the reports are contradictory. This reaction is particularly important for understanding the mechanism of alkene ozonolysis, in view of possible stabilization of reactive intermediates by aryl groups. Thus, systematic studies of ozonolysis in both aprotic solvents and in protic solvents are reported here. Attention is directed to the following details that were underestimated in the past: (i) the actual electronic structure of ground-state ozone (O3), (ii) differentiation between strained and unstrained alkenes, (iii) the significance of both the O3 concentration and the TPE concentration, (iv) the influence of various solvents, including pyridine, (v) the influence of the reaction temperature, (vi) the role of electron-transfer catalysis (ETC) and, (vii) the effect of structural modifications. Results suggest that ozonolysis of TPE (1) does not include a 1.3-dipolar reaction step, but represents a particularly interesting example of electron-donor (TPE)/electron-acceptor (O3) redox chemical The present studies include several crucial results.

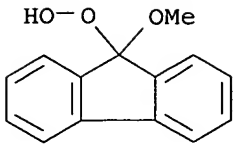
First, pure 3,3,6,6-tetraphenyltetroxane (I, m.p. 221° (dec.)) and pure tetraphenylethylene ozonide (II, m.p. 153° (dec.)) are prepared for the 1st time, although I and II have long been known. Second, the singlet diradical character of O3, lessened by hypervalent-electron interaction and predicted by different calcns., is evidenced via reaction with the spin trap galvinoxyl [2,6-bis(1,1-dimethylethyl)-4-{[3,5-bis(1,1-dimethylethyl)-4-oxocyclohexa-2,5-dien-1-ylidene]methyl}phenoxy] (8), and the zwitterionic reaction behavior of ground-state O3 is ruled out. Third, the electron-acceptor ability of O3 is evidenced by reactions with suitable tetraaryl ethylenes: it is enhanced by addition of catalytic amts. of protons or Lewis acids. Fourth, the observed distribution of the O3 O-atoms to the 2 different olefinic C-atoms of the unsym. alkene III (R = p-MeOC6H4) is in full agreement with an initial single-electron transfer (SET) step, followed by a radical mono-oxygenation to cause the crucial C,C cleavage. Final dioxygenation should lead to the generally (ozonides, tetroxanes, hydroperoxides). The regioselectivity is inconsistent with the expected decay of an intermediate primary ozonide. Finally, the treatment of 1,2-bis(4-methoxyphenyl)acenaphthylene (36) with O3 (simultaneous transfer of 3 O-atoms) leads to the same exptl. result as a stepwise transfer of one O-atom followed by a transfer of 2 O-atoms.

IT **7705-08-0**, Ferric chloride, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(electron transfer **catalyst**; electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)
RN 7705-08-0 CAPLUS
CN Iron chloride (FeCl3) (8CI, 9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **275822-22-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)
RN 275822-22-5 CAPLUS
CN Hydroperoxide, 9-methoxy-9H-fluoren-9-yl (9CI) (CA INDEX NAME)

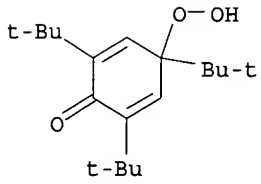


IT **7440-50-8**, Copper, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(reductive coupling **catalyst**; electron-transfer oxygenations in ozonation of 1,1,2,2-tetraphenylethene)
RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

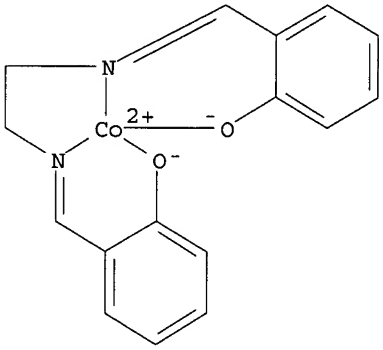
Cu

REFERENCE COUNT: 155 THERE ARE 155 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

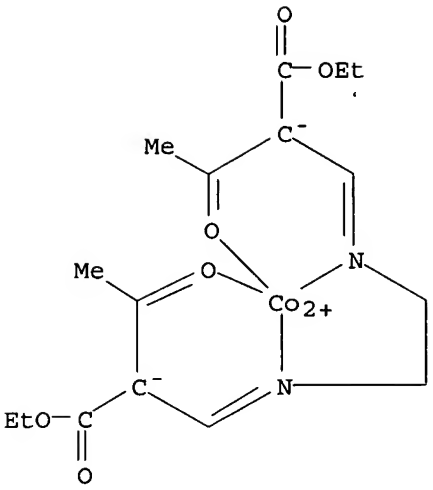
L34 ANSWER 57 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:135769 CAPLUS
DOCUMENT NUMBER: 132:250818
TITLE: Catalytic oxidation of a trialkyl-substituted phenol and aniline with biomimetic Schiff base complexes
AUTHOR(S): Knaudt, Jutta; Forster, Stefan; Bartsch, Ulrich; Rieker, Anton; Jager, Ernst-G.
CORPORATE SOURCE: Institute of Inorganic and Analytical Chemistry, University of Jena, Jena, D-07743, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2000), 55(1), 86-93
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The catalytic oxidation of 2,4,6-tri-tert-butylphenol and 2,4,6-tri-tert-butylaniline with mol. oxygen and tert-butylhydroperoxide was investigated using biomimetic Mn-, Fe- and Co-complexes as catalysts. The catalytic activity and product distribution were determined and compared with those observed in the reactions of the well-known Co(salen) complex.
IT **33919-05-0P**
RL: **BYP (Byproduct)**; **PREP (Preparation)**
(byproduct; catalytic oxidation of trialkyl-substituted phenol and aniline with biomimetic Schiff base complexes)
RN 33919-05-0 CAPLUS
CN 2,5-Cyclohexadien-1-one, 2,4,6-tris(1,1-dimethylethyl)-4-hydroperoxy- (9CI) (CA INDEX NAME)



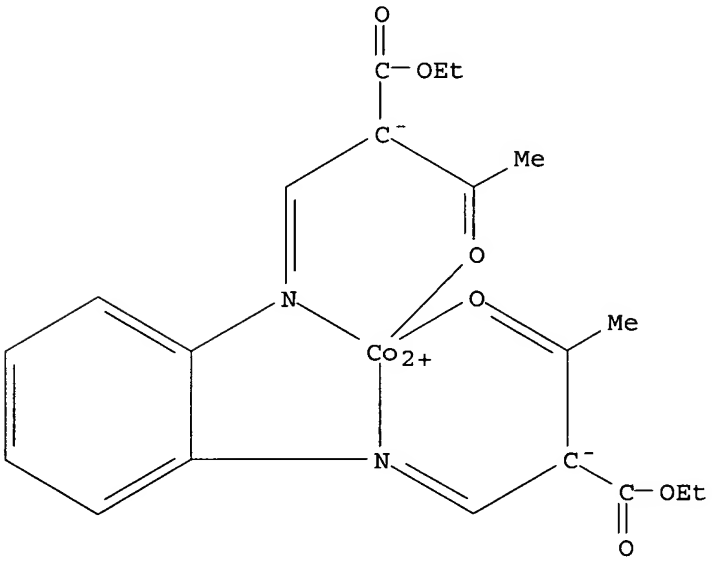
IT **14167-18-1 63510-39-4 63510-43-0**
63510-45-2 98262-52-3 99392-76-4
127899-91-6 182245-44-9
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalytic** oxidation of trialkyl-substituted phenol and aniline with biomimetic Schiff base complexes)
RN 14167-18-1 CAPLUS
CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



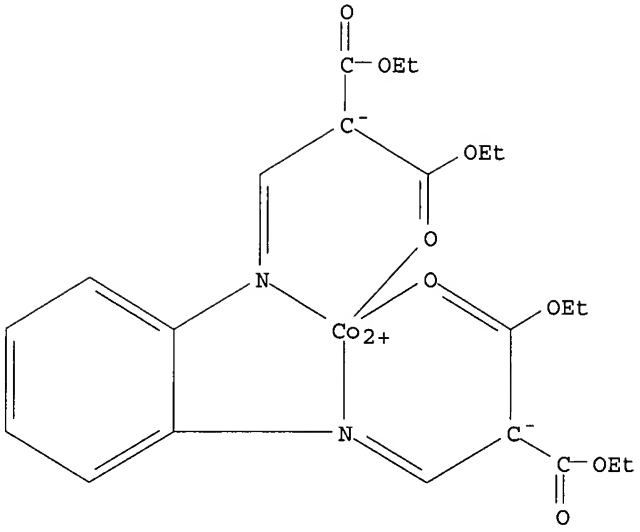
RN 63510-39-4 CAPLUS
CN Cobalt, [[diethyl 2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[3-(oxo-κO)butanoato]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



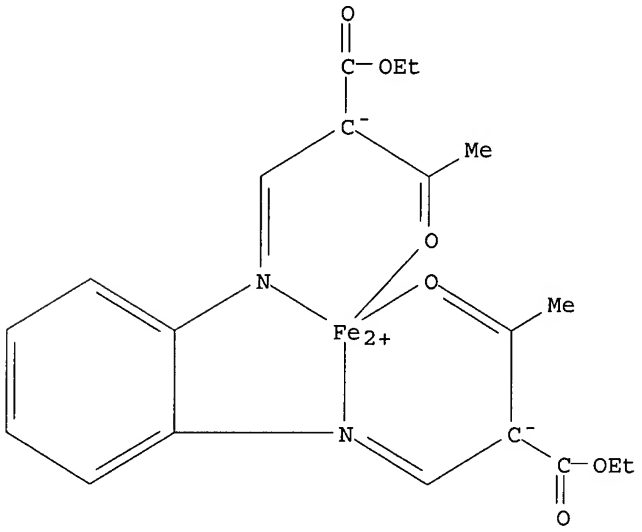
RN 63510-43-0 CAPLUS
CN Cobalt, [[diethyl 2,2'-[1,2-phenylenebis[(nitrilo-κN)methylidyne]]bis[3-(oxo-κO)butanoato]](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)



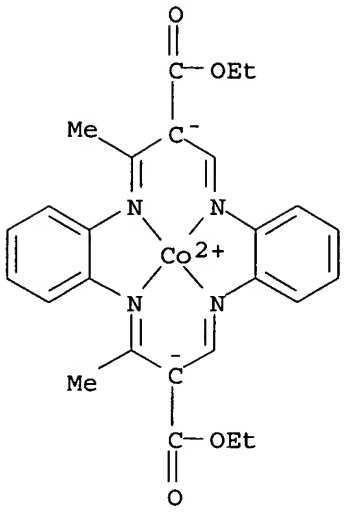
RN 63510-45-2 CAPLUS
CN Cobalt, [[tetraethyl 2,2'-[1,2-phenylenebis[(nitrilo-κN)methylidyne]]bis[propanedioato-κO1']](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)



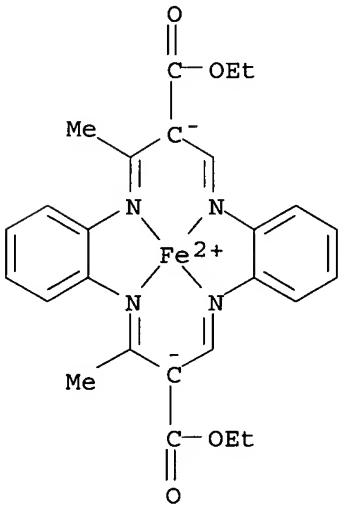
RN 98262-52-3 CAPLUS
CN Iron, [[diethyl 2,2'-[1,2-phenylenebis[(nitrilo-κN)methylidyne]]bis[3-(oxo-κO)butanoato]](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)



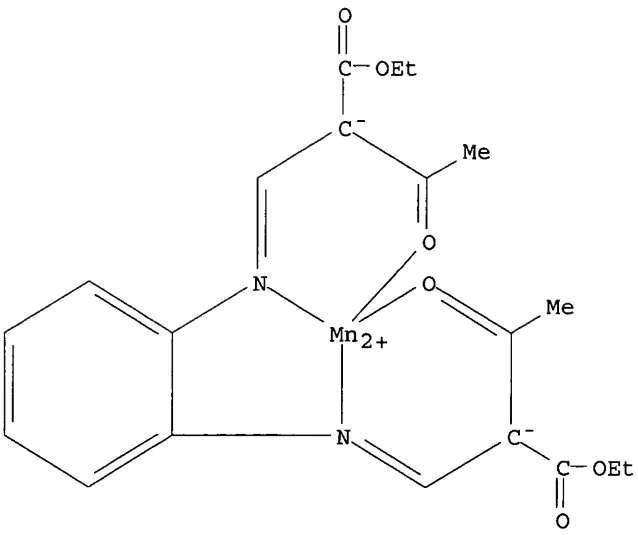
RN 99392-76-4 CAPLUS
CN Cobalt, [diethyl 7,16-dihydro-6,17-dimethyldibenzo[b,i][1,4,8,11]tetraazacyclotetradecine-7,16-dicarboxylato(2-)-κN5,κN9,κN14,.kappa.N18]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 127899-91-6 CAPLUS
CN Iron, [diethyl 7,16-dihydro-6,17-dimethyldibenzo[b,i][1,4,8,11]tetraazacyc
lotetradecine-7,16-dicarboxylato(2-)-κN5,κN9,κN14,.kappa
.N18]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 182245-44-9 CAPLUS
CN Manganese, [[diethyl 2,2'-[1,2-phenylenedi(nitrilo-κN)]bis[3-(oxo-
κO)butanoato]](2-)]- (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(catalytic oxidation of trialkyl-substituted phenol and aniline with biomimetic Schiff base complexes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O═O

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 58 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:430103 CAPLUS
DOCUMENT NUMBER: 129:110412
TITLE: Tertiary butyl alcohol absorption process for recovering propylene and isobutane in oxidation of isobutane and epoxidation of propylene
INVENTOR(S): Chess, David Durham; Pottratz, David George; Nguyen, Eileen Tovan; Culbreth, William Kemp, III
PATENT ASSIGNEE(S): Huntsman Specialty Chemicals Corp., USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5773634	A	19980630	US 1996-749190	19961114
PRIORITY APPLN. INFO.:			US 1996-749190	19961114

AB The liquid and gaseous products formed by reacting oxygen with isobutane in

an oxidation reactor are sep. processed; the liquid reaction product being charged to a distillation zone and separated into a lower boiling isobutane fraction and a higher boiling fraction comprising tert-Bu alc. and tert-Bu hydroperoxide; the gaseous reaction product comprising inert gases and vaporized and/or entrained isobutane being cooled by an amount sufficient to condense isobutane contained therein for recycle to the oxidation reactor; the remaining gases, including isobutane being charged to a tert-Bu alc. absorber to obtain a solution of isobutane in tert-Bu alc. that is recycled to the distillation zone.

IT **7439-98-7**, Molybdenum, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(epoxidn. **catalyst**; process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)
RN 7439-98-7 CAPLUS
CN Molybdenum (8CI, 9CI) (CA INDEX NAME)

Mo

IT **75-91-2P**, Tert-Butyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **PUR (Purification or recovery)**; RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)
RN 75-91-2 CAPLUS
CN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME)

HO—O—Bu-t

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for recovering propylene and isobutane by tert-Bu alc. absorption in oxidation of isobutane and epoxidn. of propylene)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

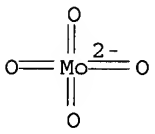
O═O

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

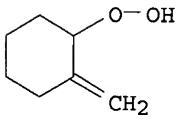
L34 ANSWER 59 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:115291 CAPLUS
DOCUMENT NUMBER: 128:179971
TITLE: Heterogeneous molybdate catalysts for the generation of singlet molecular oxygen (1Δg) from H2O2
AUTHOR(S): van Laar, F.; De Vos, D.; Vanoppen, D.; Sels, B.; Jacobs, P. A.; Del Guerzo, A.; Pierard, F.; Kirsh-De

Mesmaeker, A.
CORPORATE SOURCE: Center Surface Science and Catalysis, K. U. Leuven, Heverlee, B-3001, Belg.
SOURCE: Chemical Communications (Cambridge) (1998), (2), 267-268
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The immobilization of molybdate on Mg,Al-LDH (layered double hydroxide) leads to an active, heterogeneous catalyst that generates singlet mol. oxygen from hydrogen peroxide in the absence of soluble base. α-Terpinene, 1-methylcyclohexene, and 2,3-dimethyl-2-butene were subjected to (per)oxidation by the immobilized molybdate.

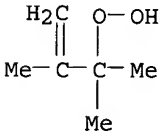
IT **14259-85-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(heterogeneous molybdate **catalysts** for generation of singlet mol. oxygen from H2O2)
RN 14259-85-9 CAPLUS
CN Molybdate (MoO42-), (T-4)- (9CI) (CA INDEX NAME)



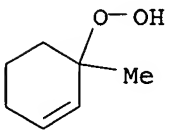
IT **4065-78-5P**, Hydroperoxide, 2-methylenecyclohexyl
13249-73-5P, Hydroperoxide, 1,1,2-trimethyl-2-propenyl
18428-16-5P, Hydroperoxide, 1-methyl-2-cyclohexen-1-yl
56595-78-9P, Hydroperoxide, 2-methyl-2-cyclohexen-1-yl
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(heterogeneous molybdate catalysts for generation of singlet mol. oxygen from H2O2)
RN 4065-78-5 CAPLUS
CN Hydroperoxide, 2-methylenecyclohexyl (7CI, 8CI, 9CI) (CA INDEX NAME)



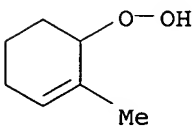
RN 13249-73-5 CAPLUS
CN Hydroperoxide, 1,1,2-trimethyl-2-propenyl (9CI) (CA INDEX NAME)



RN 18428-16-5 CAPLUS
CN Hydroperoxide, 1-methyl-2-cyclohexen-1-yl (8CI, 9CI) (CA INDEX NAME)



RN 56595-78-9 CAPLUS
CN Hydroperoxide, 2-methyl-2-cyclohexen-1-yl (9CI) (CA INDEX NAME)



IT **7782-44-7P**, Oxygen, preparation
RL: PNU (Preparation, unclassified); **RCT (Reactant)**; PREP (Preparation); **RACT (Reactant or reagent)**
(singlet; heterogeneous molybdate catalysts for generation of singlet mol. oxygen from H2O2)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 60 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:424747 CAPLUS
DOCUMENT NUMBER: 127:33911
TITLE: Preparation of mixtures of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones
INVENTOR(S): Ninomiya, Kohei; Yamamoto, Tomohiko; Umiiso, Koji; Kawai, Joji; Naito, Tatsuya
PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09143109	A2	19970603	JP 1995-309102	19951128

PRIORITY APPLN. INFO.: JP 1995-309102 19951128

AB Title mixts., useful as materials for polyamides, intermediates for chems., and organic solvents (no data), are prepared by oxidation of cycloalkanes by mol. O in the presence of Co compds. and N-hydroxydicarboximides. Cyclohexane was treated with O in the presence of N-hydroxyphthalimide and Co octylate at 160° under 10 kg/cm2G for 0.5 h to give cyclohexyl hydroperoxide, cyclohexanol, and cyclohexanone with 45.6, 26.8, and 16.4% selectivity, resp., at 3.7% conversion.

IT **6700-85-2 21679-46-9**, Cobalt tris(acetylacetonate)
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)

RN 6700-85-2 CAPLUS

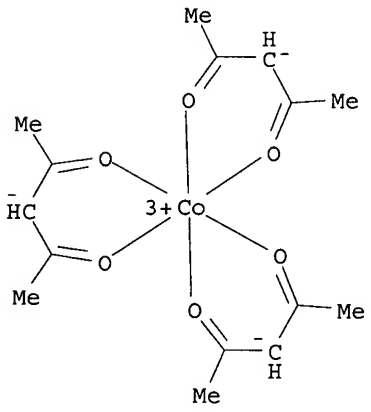
CN Octanoic acid, cobalt salt (8CI, 9CI) (CA INDEX NAME)

$HO_2C-(CH_2)_6-Me$

●x Co(x)

RN 21679-46-9 CAPLUS

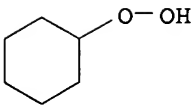
CN Cobalt, tris(2,4-pentanedionato-κO,κO')-, (OC-6-11)- (9CI) (CA INDEX NAME)



IT **766-07-4P**, Cyclohexyl hydroperoxide
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)

RN 766-07-4 CAPLUS

CN Hydroperoxide, cyclohexyl (9CI) (CA INDEX NAME)

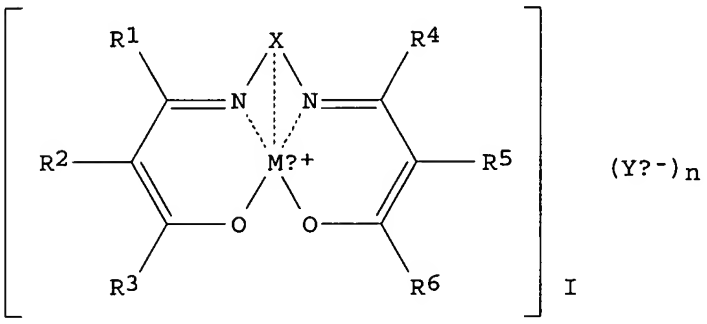


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of mixts. of cycloalkyl hydroperoxides, cycloalkanols, and cycloalkanones by oxidation of cycloalkanes with Co compds. and hydroxydicarboximides)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 61 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:320710 CAPLUS
DOCUMENT NUMBER: 126:293181
TITLE: Method for producing arylalkyl hydroperoxides
INVENTOR(S): Matsui, Narikazu; Fujita, Terunori
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09067338	A2	19970311	JP 1995-222361	19950830

PRIORITY APPLN. INFO.: JP 1995-222361 19950830
OTHER SOURCE(S): CASREACT 126:293181; MARPAT 126:293181
GI



I

AB Arylalkyl hydroperoxides represented by formula Ar[C(P)(Q)OOH]x (P, Q = H, alkyl; x = 1-3; Ar = x-valent aromatic hydrocarbon group) are prepared by oxidation of arylalkyl hydrocarbons Ar[C(P)(Q)H]x (P, Q, x = same as above) with an gas containing oxygen in the presence of a transition metal complex (e.g. I; M = transition metal having +a valences;X = atom having a lone pair electrons and forming a partial structure of a ligand together with 2 nitrogen atoms coordinating to the central metal ion; R1 - R6 = H, halo, organic group, each group being optionally linked to the adjacent organic group or forming a ring together with the adjacent organic group; Y = counter ion of -b valences; a = 2+nb, wherein 2≤a≤5 and n = 0-3). Preferably the transition metal complex is N,N'-bis(1-methyl-3-oxobutylidene)-4-aza-1,7-heptanediamine- or N,N'-disalicylidene-4-aza-1,7-heptanediamine-transition metal complex. The transition metal is selected from Mn, Co, Cu, Ni, Fe, Ta, Zr, Rh, Ru, and ions. This process uses a transition metal complex containing electron-donating atoms, i.e. N and O together with atoms selected from N, O, S, and P having lone pair electrons, and converts arylalkyl hydrocarbons into arylalkyl hydroperoxides of high concentration in high selectivity and high reaction rate using a small amount of the catalyst. Thus, 2 mg N,N'-bis(1-methyl-3-oxobutylidene)-4-aza-1,7-heptanediamine-cobalt complex was added to a mixture of 90 g cumene and 10 g cumene hydroperoxide, dissolved, and heated to 80°, followed by blowing air at 180 mL/min into the solution for 6 h to give cumene hydroperoxide at 3.1 weight%/h with 84 mol% selectivity.

IT **7439-89-6D**, Iron, complexes, uses **7440-47-3D**, Chromium, complexes, uses **14167-18-1**, [N,N'-Disalicylideneethylenediamine] cobalt **14167-20-5**, [N,N'-Disalicylideneethylenediamine]nickel **15137-09-4 33916-81-3 66328-14-1 70335-48-7 189134-24-5 189134-25-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)

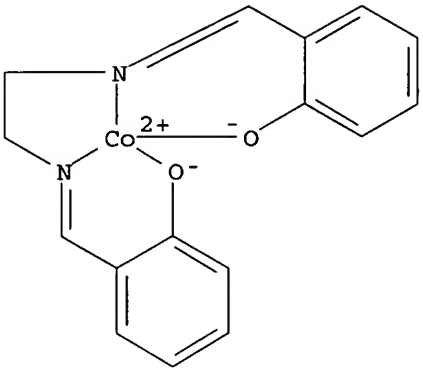
RN 7439-89-6 CAPLUS
CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)

Fe

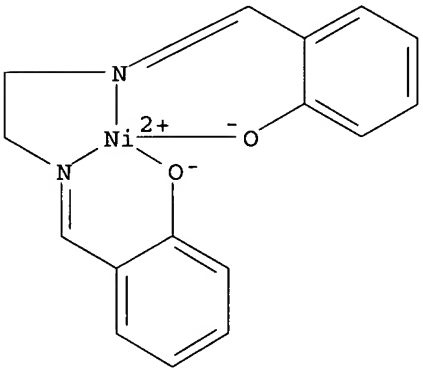
RN 7440-47-3 CAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

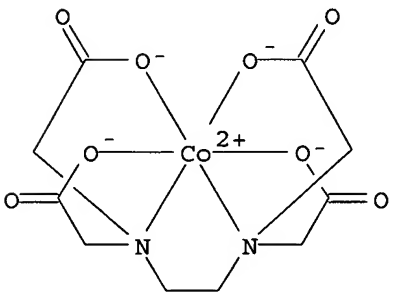
RN 14167-18-1 CAPLUS
CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 14167-20-5 CAPLUS
CN Nickel, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

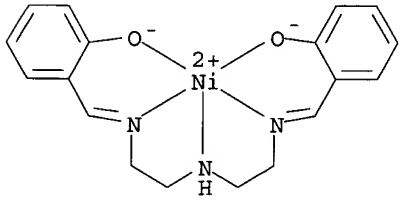


RN 15137-09-4 CAPLUS
CN Cobaltate(2-), [[N,N'-1,2-ethanediylbis[N-[(carboxy-κO)methyl]glycinato-κN,κO]](4-)]-, disodium, (OC-6-21)- (9CI) (CA INDEX NAME)

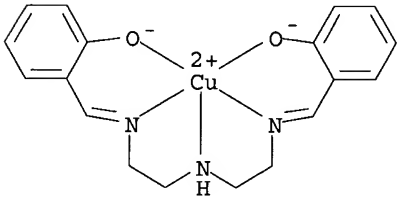


●2 Na^+

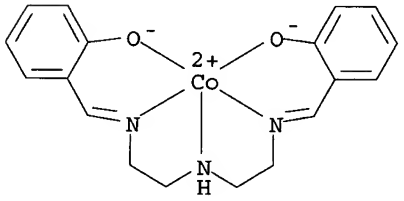
RN 33916-81-3 CAPLUS
CN Nickel, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



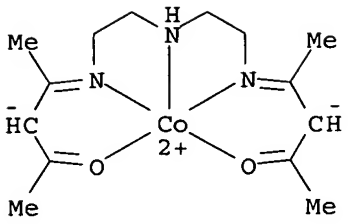
RN 66328-14-1 CAPLUS
CN Copper, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



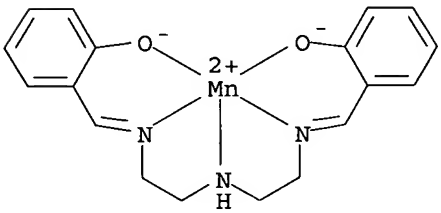
RN 70335-48-7 CAPLUS
CN Cobalt, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-5-32)- (9CI) (CA INDEX NAME)



RN 189134-24-5 CAPLUS
CN Cobalt, [[4,4'-[(imino-κN)bis(2,1-ethanediylnitrilo-κN)]bis[2-pentanonato-κO]](2-)]- (9CI) (CA INDEX NAME)

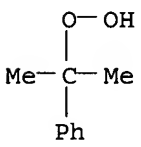


RN 189134-25-6 CAPLUS
CN Manganese, [[2,2'-[(imino-κN)bis[2,1-ethanediyl(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]- (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **80-15-9P**, Cumene hydroperoxide
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)
RN 80-15-9 CAPLUS
CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)



L34 ANSWER 62 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:320709 CAPLUS

DOCUMENT NUMBER: 126:293180
TITLE: Method for producing arylalkyl hydroperoxides
INVENTOR(S): Kagayama, Akishi; Fujita, Terunori
PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

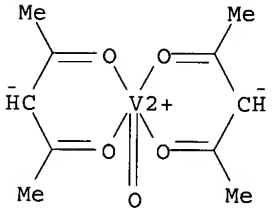
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09067337	A2	19970311	JP 1995-222360	19950830
PRIORITY APPLN. INFO.:			JP 1995-222360	19950830

OTHER SOURCE(S): CASREACT 126:293180; MARPAT 126:293180

AB Arylalkyl hydroperoxides represented by formula Ar[C(P)(Q)OOH]n (P, Q = H, alkyl; n = 1-3; Ar = n-valent aromatic hydrocarbon group) are prepared by oxidation of arylalkyl hydrocarbons Ar[C(P)(Q)H]n (P, Q, n = same as above) with an gas containing oxygen in the presence of an oxometal compound The oxometal compds. are represented by formula M(:O)Ln (M = metal; L = ligand; n = 1-8), which are preferably oxovanadium, oxotitanium, and oxozirconium compds. This process uses an oxometal compound which allows oxidation reaction at a .apprx.80° temperature range at a practical reaction rate and converts arylalkyl hydrocarbons into arylalkyl hydroperoxides of high concentration in high selectivity. Thus, 2 mg oxotitanium(II) acetylacetonate was added to a mixture of 90 g cumene and 10 g cumene hydroperoxide, and heated to 80°, followed by blowing air at 180 mL/min into the mixture for 6 h with stirring to give cumene hydroperoxide at 1.1 weight%/h and final concentration 16.9 weight% with 91 mol% selectivity.

IT **3153-26-2**, Oxovanadium(II) acetylacetonate **7440-62-2D**, Vanadium, 1,4,8,11-Tetraazacyclotetradecane complexes, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of a transition metal complexes)

RN 3153-26-2 CAPLUS
CN Vanadium, oxobis(2,4-pentanedionato-κO,κO')-, (SP-5-21)- (9CI) (CA INDEX NAME)

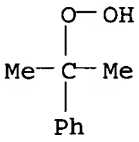


RN 7440-62-2 CAPLUS
CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of oxometal compound metal complexes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **80-15-9P**, Cumene hydroperoxide
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of arylalkyl hydroperoxides by air-oxidation of arylalkanes in presence of oxometal compound metal complexes)
RN 80-15-9 CAPLUS
CN Hydroperoxide, 1-methyl-1-phenylethyl (9CI) (CA INDEX NAME)

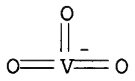


L34 ANSWER 63 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:198217 CAPLUS
DOCUMENT NUMBER: 126:277162
TITLE: Oxidations by the reagent O2-H2O2-vanadium complex-pyrazine-2-carboxylic acid. 8. Efficient oxygenation of methane and other lower alkanes in acetonitrile
AUTHOR(S): Nizova, Galina V.; Suss-Fink, Georg; Shul'pin, Georgiy B.
CORPORATE SOURCE: Semenov Inst. Chemical Physics, Russian Academy Sciences, Mowcow, 117977, Russia
SOURCE: Tetrahedron (1997), 53(10), 3603-3614
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:277162
AB All 5 C1-C4 alkanes were readily oxidized in MeCN by air and H2O2 at 20-75° using the catalytic system (n-Bu4N)VO3-pyrazine-2-carboxylic acid. Apart from alkyl hydroperoxides which are the primary oxidation products, more stable derivs. (alcs., aldehydes or ketones, and carboxylic acids) are obtained with high total turnover nos. (e.g., 420 for CH4 and 2130 for C2H6 at 75° after 4 h). In the case of ethane and cyclohexane (I), alkanes do not yield oxygenated products in the absence of air. I oxidation under 18O2 showed a high degree of 18O incorporation into the oxygenated products. Thus, H2O2 is only a promoter while O2 is the true oxidant in this oxidation
IT **76060-16-7**, Tetrabutylammonium trioxovanadate(-1)
RL: **CAT (Catalyst use)**; USES (Uses)
(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen

peroxide-vanadium complex-pyrazinecarboxylic acid reagent)
RN 76060-16-7 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, trioxovanadate(1-) (9CI) (CA INDEX NAME)

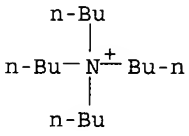
CM 1

CRN 13981-20-9
CMF O3 V
CCI CCS



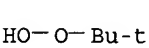
CM 2

CRN 10549-76-5
CMF C16 H36 N

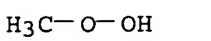


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen peroxide-vanadium complex-pyrazinecarboxylic acid reagent)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

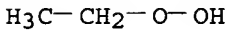
IT **75-91-2P 3031-73-0P**, Methyl hydroperoxide
3031-74-1P, Ethyl hydroperoxide **3031-75-2P**,
Hydroperoxide, 1-methylethyl **4813-50-7P**, Butyl hydroperoxide
5618-63-3P, Isobutyl hydroperoxide **6068-96-8P**,
Hydroperoxide, propyl **13020-06-9P**, sec-Butyl hydroperoxide
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(efficient oxidation of lower alkanes in acetonitrile by oxygen-hydrogen peroxide-vanadium complex-pyrazinecarboxylic acid reagent)
RN 75-91-2 CAPLUS
CN Hydroperoxide, 1,1-dimethylethyl (9CI) (CA INDEX NAME)



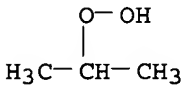
RN 3031-73-0 CAPLUS
CN Hydroperoxide, methyl (9CI) (CA INDEX NAME)



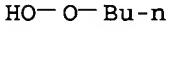
RN 3031-74-1 CAPLUS
CN Hydroperoxide, ethyl (9CI) (CA INDEX NAME)



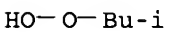
RN 3031-75-2 CAPLUS
CN Hydroperoxide, 1-methylethyl (9CI) (CA INDEX NAME)



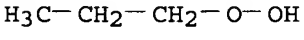
RN 4813-50-7 CAPLUS
CN Hydroperoxide, butyl (9CI) (CA INDEX NAME)



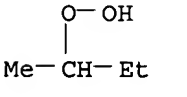
RN 5618-63-3 CAPLUS
CN Hydroperoxide, 2-methylpropyl (9CI) (CA INDEX NAME)



RN 6068-96-8 CAPLUS
CN Hydroperoxide, propyl (9CI) (CA INDEX NAME)



RN 13020-06-9 CAPLUS
CN Hydroperoxide, 1-methylpropyl (9CI) (CA INDEX NAME)



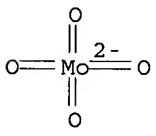
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 64 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:138298 CAPLUS
DOCUMENT NUMBER: 126:237966
TITLE: Olefin oxidation by the system H2O2/MoO42-: competition between epoxidation and peroxidation
AUTHOR(S): Nardello, Veronique; Bouttemy, Sabine; Aubry, Jean-Marie
CORPORATE SOURCE: Equipe de Recherches sur les Radicaux Libres et l'Oxygene Singulet, URA CNRS 351, Faculte de Pharmacie de Lille, BP 83, Lille, F-59006, Fr.
SOURCE: Journal of Molecular Catalysis A: Chemical (1997), 117(1-3, Proceedings of the 6th International Symposium on the Activation of Dioxygen and Homogeneous Catalytic Oxidation, 1996), 439-447
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A symposium. The oxidation of tiglic acid by the catalytic system hydrogen peroxide/molybdate ions is investigated in water under varying conditions of pH. Using similar conditions of temperature and concns., we show that two different reaction pathways compete leading either to an epoxide in acidic medium or to an allylic hydroperoxide in alkaline medium. These results are interpreted in terms of the involvement of two peroxomolybdates. Epoxidn. probably proceeds via the tetraperoxodimolybdate Mo2O3(O2)42- whereas peroxidn. involves singlet oxygen, 1O2, (1Δg), formed as a result of the decomposition of the triperoxomolybdate MoO(O2)32-. Finally, exptl. conditions are given to obtain selectively the epoxide or the hydroperoxide.

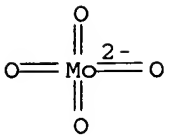
IT **7631-95-0**, Sodium molybdate **13446-49-6**, Potassium molybdate
RL: **CAT (Catalyst use)**; USES (Uses)
(epoxidn. and peroxidn. of olefins by H2O2/MoO42-)

RN 7631-95-0 CAPLUS
CN Molybdate (MoO42-), disodium, (T-4)- (9CI) (CA INDEX NAME)

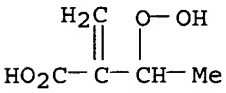


●2 Na+

RN 13446-49-6 CAPLUS
CN Molybdate (MoO42-), dipotassium, (T-4)- (9CI) (CA INDEX NAME)



IT **99268-55-0P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(epoxidn. and peroxidn. of olefins by H2O2/MoO42-)
RN 99268-55-0 CAPLUS
CN Butanoic acid, 3-hydroperoxy-2-methylene- (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: FMU (Formation, unclassified); **RCT (Reactant)**; FORM (Formation, nonpreparative); **RACT (Reactant or reagent)**
(peroxidn. of olefins by singlet oxygen formed from H2O2/MoO42-)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 65 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:218953 CAPLUS
DOCUMENT NUMBER: 127:4776
TITLE: Iron oxide colloids and t-butyl hydroperoxide in reverse microemulsions: a new and efficient system for carbon-hydrogen bond activation
AUTHOR(S): Launay, F.; Patin, H.
CORPORATE SOURCE: Lab. Chim. Organ. Substances Naturelles, CNRS URA, Rennes, 35700, Fr.
SOURCE: New Journal of Chemistry (1997), 21(2), 247-256
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Gauthier-Villars
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Iron oxide colloids generated by the hydrolysis of ferric nitrate nonahydrate in Aerosol-OT reverse microemulsions catalyze (after the addition of tert-Bu hydroperoxide) the functionalization of the hydrocarbons constituting the continuous phase of these micellar systems. In the case of cyclooctane, used to set up this new model and in all the preliminary

studies, the carbon-hydrogen bond activation products are (in decreasing order) tert-butylperoxycyclooctane, cyclooctene, cyclootanone and cyclooctanol, under static nitrogen atmospheric and at room temperature This reaction is very sensitive to temperature variations and dioxygen partial pressure. Cycloalkane tert-Bu peroxidn. remains the major process at 50°C under anaerobic conditions and makes this procedure an interesting alternative to other methods already described in the literature. The evolvement of cyclooctane oxidation into an autoxidn. reaction in the presence of mol. oxygen and model extension expts. to other substrates gave the following sequence of regioselectivity: 3°>2Å>>1°, in agreement with an homolytic cleavage of C-H bonds. The nature of the active species in such a dispersed medium is discussed on the basis of recently published results dealing with the influence of solvent polarity on tBHP decomposition

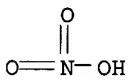
IT **1317-60-8**, Hematite, uses
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(colloidal α-; iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

RN 1317-60-8 CAPLUS
CN Hematite (Fe2O3) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	3	17778-80-2
Fe	2	7439-89-6

IT **7782-61-8**, Ferric nitrate nonahydrate **10421-48-4**, Ferric nitrate
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)

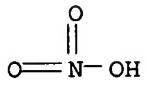
RN 7782-61-8 CAPLUS
CN Nitric acid, iron(3+) salt, nonahydrate (9CI) (CA INDEX NAME)



●1/3 Fe(III)

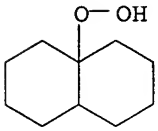
●3 H_2O

RN 10421-48-4 CAPLUS
CN Nitric acid, iron(3+) salt (8CI, 9CI) (CA INDEX NAME)

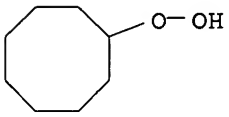


●1/3 Fe(III)

IT **4181-83-3P 5130-47-2P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)
RN 4181-83-3 CAPLUS
CN Hydroperoxide, octahydro-4a(2H)-naphthalenyl (9CI) (CA INDEX NAME)



RN 5130-47-2 CAPLUS
CN Hydroperoxide, cyclooctyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**; USES (Uses)
(radical trap; iron oxide colloids and t-Bu hydroperoxide in reverse microemulsions as efficient system for carbon-hydrogen bond activation)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 66 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:133466 CAPLUS
DOCUMENT NUMBER: 126:224918
TITLE: Oxygen activation by metal complexes and alkyl

hydroperoxides. Applications of mechanistic probes to explore the role of alkoxyl radicals in alkane functionalization

AUTHOR(S): MacFaul, Philip A.; Arends, Isabella W. C. E.; Ingold, Keith U.; Wayner, Danial D. M.

CORPORATE SOURCE: Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON, K1A OR6, Can.

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1997), (2), 135-145
CODEN: JCPKBH; ISSN: 0300-9580

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides catalyzed by iron(III) dichlorotris(2-pyridylmethyl)amine [FeIIICl2(TPA)]+ and by the acetate bridged (μ-oxo) di-iron complex [Fe2III(TPA)2O(OAc)]3+ has been investigated. Product studies do not support oxidation via a high valent iron-oxo intermediate (formally FeV:O), but are consistent with a mechanism involving hydrogen atom abstraction from the alkane by alkoxyl radicals derived from the hydroperoxide. In the presence of a large excess of tert-Bu hydroperoxide, the oxidation of cyclohexane yields cyclohexanone, cyclohexanol and tert-Bu cyclohexyl peroxide in more than stoichiometric amts. and, in the case of the mono-iron catalyst, one equivalent of cyclohexyl chloride. Replacement of Me3COOH by hydroperoxides which could yield tert-alkoxyl radicals having much shorter lifetimes than the tert-butoxyl radical prevents oxidation of the cycloalkane. The products obtained with these hydroperoxide mechanistic probes are those derived from the fast unimol. reactions (generally β-scissions) of the corresponding alkoxyl radicals. The inapplicability of di-Me sulfide as a mechanistically diagnostic trap for the putative FeV:O intermediate and the value of di-tert-Bu hyponitrite as a non-iron-based source of tert-butoxyl radicals are discussed.

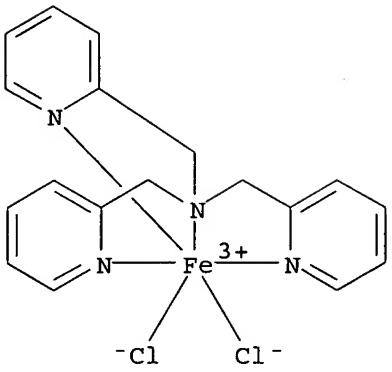
IT **128412-29-3 164223-84-1 188175-48-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides **catalyzed** by iron(III) complexes)

RN 128412-29-3 CAPLUS

CN Iron(1+), [N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]dichloro-, (OC-6-32)-, perchlorate (9CI) (CA INDEX NAME)

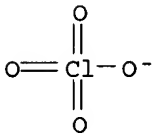
CM 1

CRN 128412-28-2
CMF C18 H18 Cl2 Fe N4
CCI CCS



CM 2

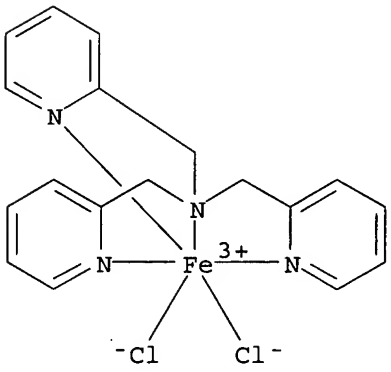
CRN 14797-73-0
CMF Cl O4



RN 164223-84-1 CAPLUS
CN Iron(1+), [N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]dichloro-, (OC-6-32)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

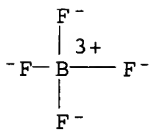
CM 1

CRN 128412-28-2
CMF C18 H18 Cl2 Fe N4
CCI CCS



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

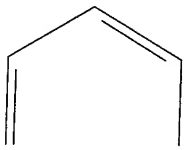


RN 188175-48-6 CAPLUS
CN Iron(3+), [μ-(acetato-κO:κO')]bis[N,N-bis[(2-pyridinyl-κN)methyl]-2-pyridinemethanamine-κN1,κN2]-μ-oxodi-, stereoisomer, tris[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

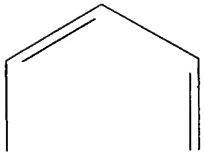
CM 1

CRN 121757-78-6
CMF C38 H39 Fe2 N8 O3
CCI CCS

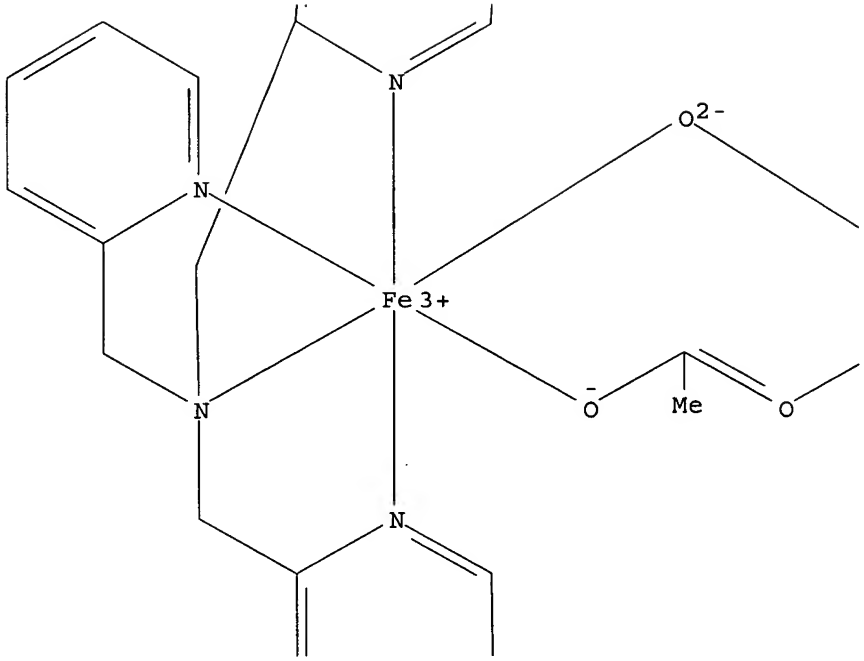
PAGE 1-A



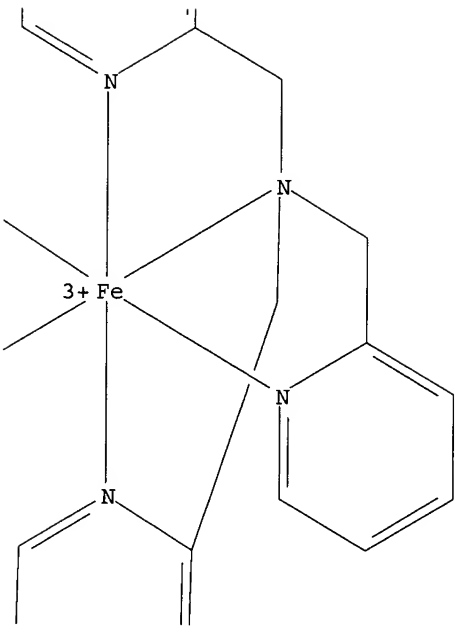
PAGE 1-B



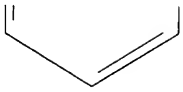
PAGE 2-A



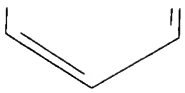
PAGE 2-B



PAGE 3-A

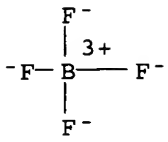


PAGE 3-B



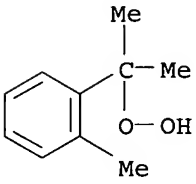
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



IT **7782-44-7**, Oxygen, reactions
RL: PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides catalyzed by iron(III) complexes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **13387-56-9P**, o-Methylcumene hydroperoxide
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; PROC (Process); RACT (Reactant or reagent)
(mechanism of the oxidation of cycloalkanes by tertiary alkyl hydroperoxides catalyzed by iron(III) complexes)
RN 13387-56-9 CAPLUS
CN Hydroperoxide, 1-methyl-1-(2-methylphenyl)ethyl (9CI) (CA INDEX NAME)



REFERENCE COUNT: 101 THERE ARE 101 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 67 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:603937 CAPLUS
DOCUMENT NUMBER: 123:111661
TITLE: Process for production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide
INVENTOR(S): Ikimi, Kiyoshi; Ikeda, Yoichi; Murakami, Akira; Okamoto, Kazushige; Tokumaru, Tooru; Hazama, Motoo
PATENT ASSIGNEE(S): Suitomo Chemical Co., Ltd., Japan
SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 10,837, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5399791	A	19950321	US 1994-202160	19940225
JP 05208928	A2	19930820	JP 1992-16136	19920131
JP 3537455	B2	20040614		

PRIORITY APPLN. INFO.: JP 1992-16136 A 19920131
US 1993-10837 B2 19930129

OTHER SOURCE(S): CASREACT 123:111661; MARPAT 123:111661

AB A process for the production of cresols, comprising the steps of: (a) conducting oxygenation of cymene with oxygen gas or an oxygen-containing gas without any addition of an alkali, thereby obtaining a solution of oxygenation products containing tertiary and primary hydroperoxides of cymene; (b) washing the solution of oxygenation products obtained in step (a) with an aqueous alkali solution at a temperature in the range of from 10° to 95°, said aqueous alkali solution having a concentration of 0.1 to 2.0 weight %, and the weight ratio of the aqueous alkali solution to the solution of oxygenation products being in the range of from 1/5 to 1/15 (weight/weight); (c) subjecting the solution of oxygenation products obtained in step (b) to hydrogenation at a temperature in the range of from 60° to 100° to decrease the content of primary hydroperoxide in such a manner that the weight ratio of primary hydroperoxide to tertiary hydroperoxide is not greater than 1/25 (weight/weight); (d) subjecting the solution treated in step (c) to decomposition in the presence of a catalyst; and (e) subjecting the solution treated in step (d) to hydrogenation to obtain cresols. Thus, e.g., oxidation of cymene (807.0 g; content, 99.3%) and a cymene solution [78.0 g; cymene content, 82.1%; tertiary hydroperoxide (3HPO) content, 11.2%; and 1HPO content, 0.65%] containing cymene hydroperoxide with air afforded 909.2 g of a hydroperoxide mixture-containing oil phase (composition: cymene, 81.9%; 3HPO, 12.1%; 1HPO, 2.2% + others); hydrogenation over 1% palladium-titania catalyst afforded 909.2 g of the reaction mixture (composition: cymene, 81.8%; 3HPO, 11.0%; 1HPO, 0.03% + others) in which the weight ratio of 1HPO to 3HPO is 1/370, and the degree of conversion is 98.7% for 1HPO and 8.7% for 3HPO, resp.; from this reaction mixture, the unreacted portion (699.8 g) of cymene is removed by distillation, 209.3 g of the concentrate is obtained (composition: cymene, 21.0%; 3HPO, 47.8%; 1HPO, 0.13%); decomposition of the mixture in presence of sulfuric acid (0.17 g) and acetone (29 g) afforded a 238.3 g solution of decomposition products (composition: cymene, 18.3%; 3HPO, not found; 1HPO, not found; cresol, 26.0%; + others) with the yield of cresol from consumed cymene = 59.4%; hydrogenation of decomposition products over 1% palladium-titania afforded 63.0 g of cresol and 82.1 g of cymene, with the yield of cresol from consumed cymene = 86%. When the first hydrogenation step was omitted, the yield of cresol from consumed cymene is 72.8%.

IT **7440-47-3**, Chromium, uses **7440-50-8**, Copper, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(copper-chromium **catalysts**; production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)

RN 7440-47-3 CAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

IT **7440-02-0**, Nickel, uses **7440-02-0D**, Nickel,
1,2-Diphenyl-1,2-ethenedithiol complexes **7440-50-8D**, Copper,
1,2-Diphenyl-1,2-ethenedithiol complexes **12026-57-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)
RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

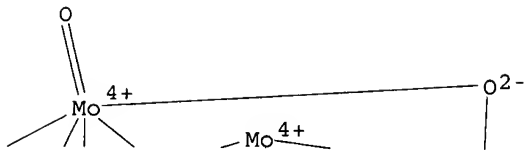
Ni

RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

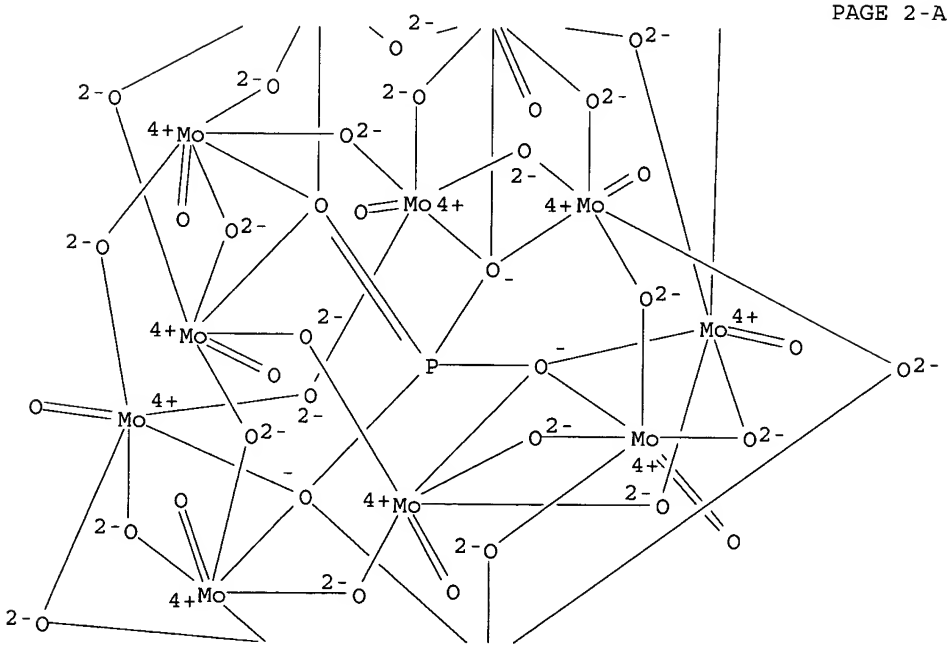
Cu

RN 12026-57-2 CAPLUS
CN Molybdate(3-), tetracosa-μ-oxododecaoxo[μ12-[phosphato(3-)-κO:κO:κO:κO':κO':κO':κO'':.kappa.O'':κO'':κO''':κO''':κO''']]dodeca-, trihydrogen (9CI) (CA INDEX NAME)

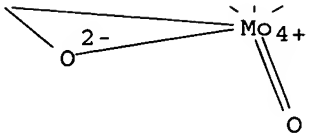
PAGE 1-A

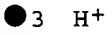


PAGE 2-A



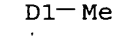
PAGE 3-A

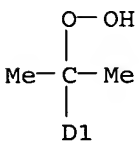




IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **26444-17-7P**, Cymene hydroperoxide
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(production of cresols via oxygenation of cymene and selective removal of cymene primary hydroperoxide)
RN 26444-17-7 CAPLUS
CN Hydroperoxide, 1-methyl-1-(methylphenyl)ethyl (9CI) (CA INDEX NAME)





L34 ANSWER 68 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:606901 CAPLUS
DOCUMENT NUMBER: 123:9156

TITLE: Process and catalysts for producing aromatic peroxycarboxylic acids from aromatic aldehydes
INVENTOR(S): Oda, Yoshiaki
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 653420	A1	19950517	EP 1994-117863	19941111
EP 653420	B1	19980311		
R: DE, FR, GB, IT, NL				
JP 07188161	A2	19950725	JP 1994-244284	19941007
US 5523468	A	19960604	US 1994-341901	19941115
PRIORITY APPLN. INFO.:			JP 1993-286607 A	19931116
			JP 1994-244284 A	19941007

OTHER SOURCE(S): CASREACT 123:9156

AB Aromatic peroxycarboxylic acids (e.g., PhCO2OH) are prepared in high yield, without significant product decomposition, by reacting an aromatic aldehyde (e.g., PhCHO) and O2(g) in the presence of ≥1 transition metal oxide(s), selected from Cr, Mn, Fe, Co, Ni, and Cu, in a solvent (e.g., C6H6).

IT **1308-06-1**, Cobalt oxide (Co3O4) **1308-38-9**, Chromium oxide (Cr2O3), uses **1309-37-1**, Ferric oxide, uses **1313-13-9**, Manganese IV oxide, uses **1314-06-3**, Nickel oxide (Ni2O3) **1317-38-0**, Cupric oxide, uses **1317-39-1**, Cuprous oxide, uses **1317-61-9**, Iron oxide (Fe3O4), uses **1345-25-1**, Ferrous oxide, uses **7439-89-6D**, Iron, oxides **7439-96-5D**, Manganese, oxides **7440-02-0D**, Nickel, oxides **7440-47-3D**, Chromium, oxides **7440-48-4D**, Cobalt, oxides **7440-50-8D**, Copper, oxides
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts** for producing aromatic peroxycarboxylic acids from aromatic aldehydes)

RN 1308-06-1 CAPLUS
CN Cobalt oxide (Co3O4) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 1308-38-9 CAPLUS
CN Chromium oxide (Cr2O3) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 1309-37-1 CAPLUS
CN Iron oxide (Fe2O3) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 1313-13-9 CAPLUS
CN Manganese oxide (MnO2) (8CI, 9CI) (CA INDEX NAME)

O═Mn═O

RN 1314-06-3 CAPLUS

CN Nickel oxide (Ni2O3) (6CI, 8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 1317-38-0 CAPLUS
CN Copper oxide (CuO) (8CI, 9CI) (CA INDEX NAME)

Cu═O

RN 1317-39-1 CAPLUS
CN Copper oxide (Cu2O) (8CI, 9CI) (CA INDEX NAME)

Cu—O—Cu

RN 1317-61-9 CAPLUS
CN Iron oxide (Fe3O4) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 1345-25-1 CAPLUS
CN Iron oxide (FeO) (8CI, 9CI) (CA INDEX NAME)

Fe═O

RN 7439-89-6 CAPLUS
CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)

Fe

RN 7439-96-5 CAPLUS
CN Manganese (8CI, 9CI) (CA INDEX NAME)

Mn

RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-47-3 CAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

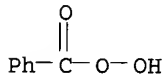
RN 7440-48-4 CAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

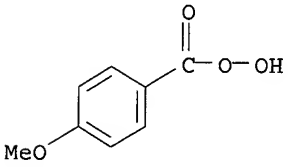
RN 7440-50-8 CAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

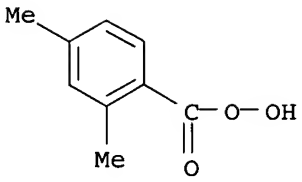
IT **93-59-4P**, Peroxybenzoic acid **940-10-3P**, 4-Methoxyperoxybenzoic acid **123088-67-5P**, Benzenecarboperoxoic acid, 2,4-Dimethyl-
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(process and catalysts for producing aromatic peroxycarboxylic acids from aromatic aldehydes)
RN 93-59-4 CAPLUS
CN Benzenecarboperoxoic acid (9CI) (CA INDEX NAME)



RN 940-10-3 CAPLUS
CN Benzenecarboperoxoic acid, 4-methoxy- (9CI) (CA INDEX NAME)

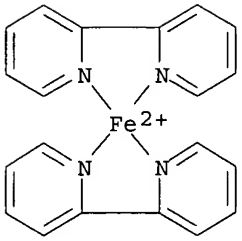


RN 123088-67-5 CAPLUS
CN Benzenecarboperoxoic acid, 2,4-dimethyl- (9CI) (CA INDEX NAME)

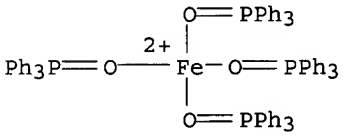


IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process and catalysts for producing aromatic peroxycarboxylic acids from aromatic aldehydes)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 69 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:988670 CAPLUS
DOCUMENT NUMBER: 124:175160
TITLE: Iron(II)-Induced Activation of Dioxygen for Oxygenation of Cyclohexene and Methyl Linoleate and Initiation of the Autoxidation of 1,4-Cyclohexadiene
AUTHOR(S): Hage, John P.; Powell, John A.; Sawyer, Donald T.
CORPORATE SOURCE: Department of Chemistry, Texas A and M University, College Station, TX, 77843-3255, USA
SOURCE: Journal of the American Chemical Society (1995), 117(51), 12897-8
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB FeII(byp)22+ and FeII(OPPh3)42+ in MeCN catalytically activate O2 for the direct oxygenation of cyclohexene of Me linoeate. The FeII(byp)22+/O2/MeCN system initiated the autoxidn. of 1,4-cyclohexadiene and PhCHO.
IT **15552-69-9** **47921-14-2**
RL: **CAT (Catalyst use)**; NUU (Other use, unclassified); USES (Uses)
(iron(II)-induced activation of dioxygen for oxygenation of cyclohexene and Me linoleate)
RN 15552-69-9 CAPLUS
CN Iron(2+), bis(2,2'-bipyridine-κN1,κN1')- (9CI) (CA INDEX NAME)

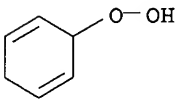


RN 47921-14-2 CAPLUS
CN Iron(2+), tetrakis(triphenylphosphine oxide-κO)-, (T-4)- (9CI) (CA INDEX NAME)



IT **7782-44-7**, Dioxygen, reactions
RL: PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(iron(II)-induced activation of dioxygen for oxygenation of cyclohexene and Me linoleate)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

IT **173910-76-4P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(iron(II)-initiated autoxidn. of 1,4-cyclohexadiene and PhCHO)
RN 173910-76-4 CAPLUS
CN Hydroperoxide, 2,5-cyclohexadien-1-yl (9CI) (CA INDEX NAME)



L34 ANSWER 70 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:213711 CAPLUS
DOCUMENT NUMBER: 116:213711
TITLE: Carbon dioxide as modulator of the oxidative properties of dioxygen in the presence of transition metal systems

AUTHOR(S): Aresta, Michele; Fragale, Carlo; Quaranta, Eugenio; Tommasi, Immacolata
CORPORATE SOURCE: Dip. Chim., CNR, Bari, 70126, Italy
SOURCE: Journal of the Chemical Society, Chemical Communications (1992), (4), 315-17
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:213711

AB In the presence of transition metal (Fe, Rh) catalysts, CO2 can modulate the oxidative properties of O2 towards THF (THF) and styrene; the intermediate formation of metal-peroxocarbonate species, seems to play a key role in these processes. E.g., oxidation of THF by O2 in the presence of FeCl2 gave 2-hydroxytetrahydrofuran (I), butyrolactone (II), succinic anhydride, and succinaldehyde. Use of CO2-O2 (1:1 by volume) gave I and II selectively.

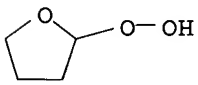
IT **7758-94-3**, Iron dichloride
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalyst**, for oxidation of THF in presence of carbon dioxide)
RN 7758-94-3 CAPLUS
CN Iron chloride (FeCl2) (8CI, 9CI) (CA INDEX NAME)

Cl—Fe—Cl

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation by, of organic substrates, effect of carbon dioxide on)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O═O

IT **4676-82-8P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of, by oxidation of THF, catalytic)
RN 4676-82-8 CAPLUS
CN Hydroperoxide, tetrahydro-2-furanyl (9CI) (CA INDEX NAME)



L34 ANSWER 71 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:435485 CAPLUS
DOCUMENT NUMBER: 117:35485
TITLE: Application of air electrode
AUTHOR(S): Wu, Zhiyuan; Li, Shengxian
CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, Peop. Rep. China
SOURCE: Wuhan Daxue Xuebao, Ziran Kexueban (1991), (3), 99-104

CODEN: WTHPDI; ISSN: 0253-9888
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB Alkaline solution of hydrogen peroxide can be prepared by electroredn. of oxygen on porous gas cathodes in caustic medium. The current efficiency and cathode lifetime depends on the condition of electrolysis. Exptl. results show that continuous operative lifetimes of the electrode can be longer than 2000 h at c.d. of 50 mA/cm2. The electrode is applied to preparation of oxygen by placing a MnO2 covered iron screen in the cell. The number of coulombs required for generating same oxygen vols. is discussed.

IT **1308-06-1**, Cobalt oxide (Co3O4) **1313-13-9**, Manganese dioxide, uses **12017-35-5**, Cobalt nickel oxide (Co2NiO4)
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalyst**, for decomposition of hydrogen peroxide)

RN 1308-06-1 CAPLUS
CN Cobalt oxide (Co3O4) (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 1313-13-9 CAPLUS
CN Manganese oxide (MnO2) (8CI, 9CI) (CA INDEX NAME)

O═Mn═O

RN 12017-35-5 CAPLUS
CN Cobalt nickel oxide (Co2NiO4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Co	2	7440-48-4
Ni	1	7440-02-0

IT **14691-59-9P**, Peroxide (HO21-)
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in electrochem. reduction of oxygen)

RN 14691-59-9 CAPLUS
CN Peroxide (HO21-) (8CI, 9CI) (CA INDEX NAME)

$^{-}$O—OH

IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reduction of, electrochem., on porous gas electrode in alkaline medium, hydrogen peroxide production from)

RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

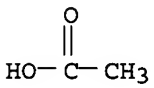
O═O

L34 ANSWER 72 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:517196 CAPLUS
DOCUMENT NUMBER: 111:117196
TITLE: Catalytic oxidation of cyclohexene by oxygen
AUTHOR(S): Belov, P. S.; Nizova, S. A.; Fedorova, R. I.; Mitina, V. v.; Pleshivtseva, A. V.
CORPORATE SOURCE: Mosk. Inst. Nefti Gaza im Gubkina, Moscow, USSR
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1989), 62(2), 353-7
CODEN: ZPKHAB; ISSN: 0044-4618
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Selectivity of the oxidation of cyclohexene (I) by O to 1,2-epoxycyclohexane (II) and 2,3-epoxy-1-cyclohexanol (III) in the presence of the catalysts Cu(OAc)2, Co/zeolite, V2 (a V-containing catalyst), VO(acac)2 (acac = acetylacetonate), Mo(CO)6, and their mixts. was studied in an attempt to obtain II and III without introduction of cyclohexenyl hydroperoxide (IV) into the reaction mixture I oxidation in the presence of Cu(OAc)2, Co/zeolite, or V2 gave IV as the main product with II and III obtained in insignificant amts., whereas selectivity for II and III was relatively high with minor IV formation in oxidation in the presence of VO(acac)2 or Mo(CO)6. The highest yields of II and III for binary catalyst systems were obtained by simultaneous introduction of V2 and VO(acac)2 into the reaction mixture at a 1:1 ratio. For ternary catalyst systems, the highest yields were obtained by I oxidation in the presence of 6:1:1 Co/zeolite-VO(acac)2-Mo(CO)6 systems.

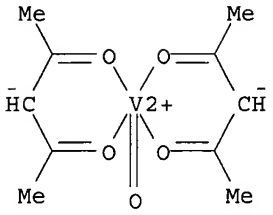
IT **142-71-2**, Copper diacetate **3153-26-2**, Oxobis(acetylacetonato)vanadium **7440-62-2**, Vanadium, uses and miscellaneous **13939-06-5**, Molybdenum hexacarbonyl
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts**, for oxidation of cyclohexene to epoxycyclohexane and epoxycyclohexanol, selectivity of)

RN 142-71-2 CAPLUS
CN Acetic acid, copper(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Cu(II)

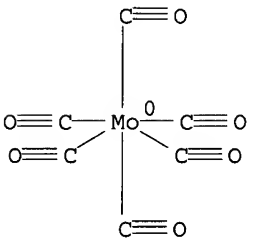
RN 3153-26-2 CAPLUS
CN Vanadium, oxobis(2,4-pentanedionato-κO,κO')-, (SP-5-21)- (9CI) (CA INDEX NAME)



RN 7440-62-2 CAPLUS
CN Vanadium (8CI, 9CI) (CA INDEX NAME)

V

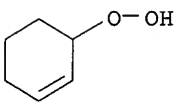
RN 13939-06-5 CAPLUS
CN Molybdenum carbonyl (Mo(CO)6), (OC-6-11)- (9CI) (CA INDEX NAME)



IT **7440-48-4**, Cobalt, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts**, zeolite-supported, for oxidation of cyclohexene to epoxycyclohexane and epoxycyclohexanol, selectivity of)
RN 7440-48-4 CAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT **4845-05-0P**
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in cyclohexene oxidation to epoxycyclohexane and epoxycyclohexanol, effect of catalyst selectivity on)
RN 4845-05-0 CAPLUS
CN Hydroperoxide, 2-cyclohexen-1-yl (9CI) (CA INDEX NAME)



IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation by, of cyclohexene, to epoxycyclohexane and epoxycyclohexanol, catalysts for, selectivity of)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 73 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:123602 CAPLUS
DOCUMENT NUMBER: 110:123602
TITLE: Kinetic study of oxygen reduction to HO2- on teflon-bonded copper manganite electrodes
AUTHOR(S): Gautier, J. L.; Restovic, A.; Chartier, P.
CORPORATE SOURCE: Fac. Cienc., Univ. Santiago, Santiago, Chile
SOURCE: Boletin de la Sociedad Chilena de Quimica (1988), 33(4), 209-27
CODEN: BOCQAX; ISSN: 0366-1644
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
AB O2 is electrocatalytically reducible in alkaline medium on Teflon-bonded Cu1+xMn2-xO4 electrodes showing spinel structure. The reduction is likely to occur on active Mn sites through HO2- formation. A mechanism for the electroredn. of O2 is proposed according to exptl. kinetics parameters. In the region of low degrees of polarization the protonation of O2- seems the rate-determining step, whereas at high overpotentials the addition of the first electron to adsorbed O2 is considered the rate-determining step. The influence of the tri- and tetravalent cations in the structure on the kinetics and reactions scheme is shown.
IT **12019-04-4**, Copper manganese oxide (CuMn2O4) **56320-15-1**, Copper manganese oxide (Cu1.2Mn1.8O4) **62975-03-5**, Copper manganese oxide (Cu1.4Mn1.6O4) **119398-08-2**, Copper manganese oxide (Cu1.3Mn1.7O4) **119398-10-6**, Copper manganese oxide (Cu1.1Mn1.9O4)
RL: PRP (Properties)
(**electrocatalyst**, Teflon-bonded, for oxygen reduction in alkaline solution)
RN 12019-04-4 CAPLUS
CN Copper manganese oxide (CuMn2O4) (8CI, 9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1	7440-50-8
Mn	2	7439-96-5

RN 56320-15-1 CAPLUS
CN Copper manganese oxide (Cu1.2Mn1.8O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number

O	4	17778-80-2
Cu	1.2	7440-50-8
Mn	1.8	7439-96-5

RN 62975-03-5 CAPLUS
CN Copper manganese oxide (Cu1.4Mn1.6O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.4	7440-50-8
Mn	1.6	7439-96-5

RN 119398-08-2 CAPLUS
CN Copper manganese oxide (Cu1.3Mn1.7O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.3	7440-50-8
Mn	1.7	7439-96-5

RN 119398-10-6 CAPLUS
CN Copper manganese oxide (Cu1.1Mn1.9O4) (9CI) (CA INDEX NAME)

Component	Ratio	Component Registry Number
O	4	17778-80-2
Cu	1.1	7440-50-8
Mn	1.9	7439-96-5

IT **14691-59-9P**, Peroxide (HO21-)
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in electrocatalytic reduction of oxygen on Teflon-bonded copper manganate)
RN 14691-59-9 CAPLUS
CN Peroxide (HO21-) (8CI, 9CI) (CA INDEX NAME)

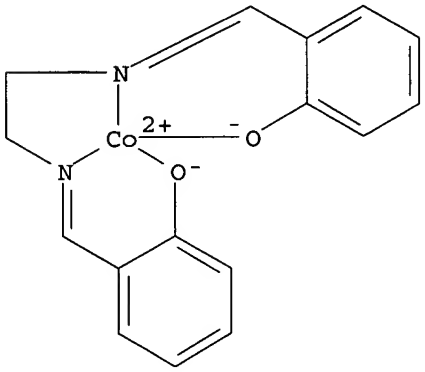
IT **7782-44-7**, Oxygen, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reduction of, copper manganate electrocatalyst bonded with Teflon for)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 74 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:174353 CAPLUS
DOCUMENT NUMBER: 100:174353
TITLE: Oxygenation of olefins under reductive conditions. Cobalt-catalyzed selective conversion of aromatic olefins to benzylic alcohols by molecular oxygen and tetrahydroborate
AUTHOR(S): Okamoto, Tadashi; Oka, Shinzaburo
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan
SOURCE: Journal of Organic Chemistry (1984), 49(9), 1589-94
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

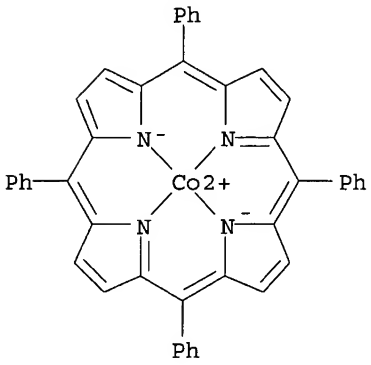
AB A high-yield catalytic conversion of RC6H4CR1:CHR2 (R = H, 4-Cl, 2-, 4-Me, 4-MeO, 4-Br, 3-O2N; R1 = H, Me; R2 = H, Me, CH2OH, CH:CH2, CH2CH:CH2, CH2CH2CH:CH2) to benzylic alcs. RC6H4CR1(OH)CH2R2 (I) by mol. O2 and BH4- was catalyzed by Co(TPP) (TPP = tetraphenylporphyrin). The reaction was regioselective exclusively. Comparison of the product distribution and D incorporation in the catalytic oxygenation of PhCH:CH2, the stoichiometric oxygenation of alkylcobalt complex PhCHMeCoLR32 (II; L = pyridine, R3 = dimethylglyoxime anion) and the decomposition of hydroperoxide PhCHMeOOH (III) indicated III was the primary product. III was formed by the reaction of II with mol. O2. Co(TPP) catalyzed 3 reactions in the overall catalytic process: formation of III, decomposition of III to benzylic alc. and aryl ketone, and reduction of the ketone.

IT **7782-44-7**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation by, of aromatic olefins, benzyl alcs. by, cobalt tetraphenylporphyrin catalyzed)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

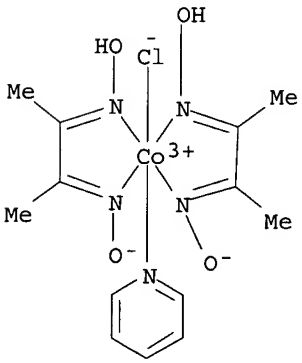
IT **14167-18-1 14172-90-8 23295-32-1 37115-10-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation **catalyst**, for aromatic olefin to benzyl alcs.)
RN 14167-18-1 CAPLUS
CN Cobalt, [[2,2'-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[phenolato-κO]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



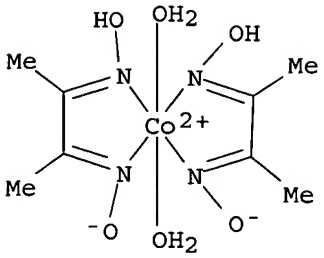
RN 14172-90-8 CAPLUS
CN Cobalt, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



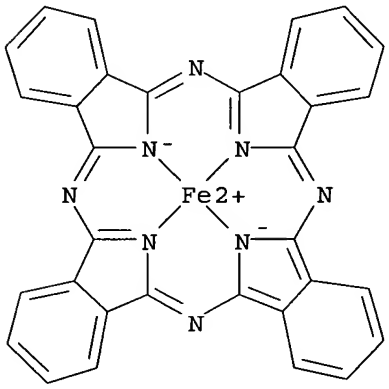
RN 23295-32-1 CAPLUS
CN Cobalt, bis[[2,3-butanedione di(oximato-κN)](1-)]chloro(pyridine)-, (OC-6-42)- (9CI) (CA INDEX NAME)



RN 37115-10-9 CAPLUS
CN Cobalt, diaquabis[[2,3-butanedione di(oximato-κN)](1-)]-, (OC-6-12)- (9CI) (CA INDEX NAME)



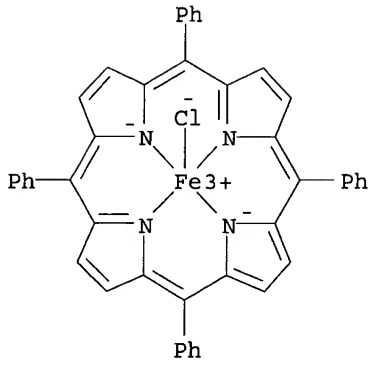
IT **132-16-1 7646-79-9**, uses and miscellaneous
16456-81-8 19973-61-6 89556-84-3
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation **catalyst**, for aromatic olefins to benzyl alcs.)
RN 132-16-1 CAPLUS
CN Iron, [29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,.kapp
a.N32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



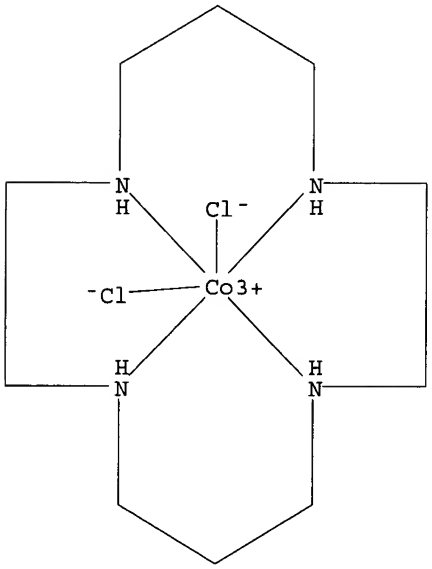
RN 7646-79-9 CAPLUS
CN Cobalt chloride (CoCl2) (8CI, 9CI) (CA INDEX NAME)

Cl—Co—Cl

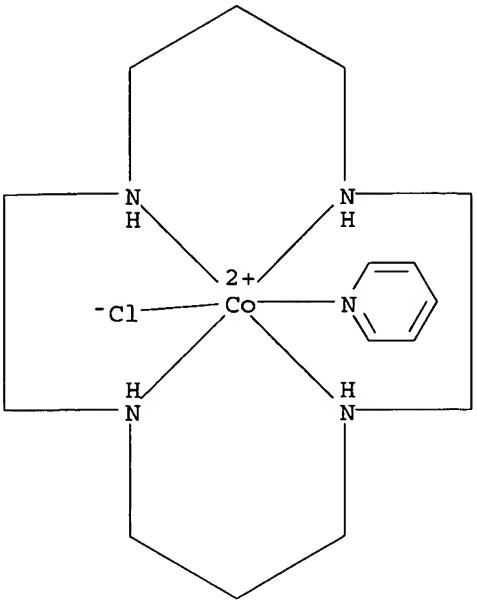
RN 16456-81-8 CAPLUS
CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-
κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX
NAME)



RN 19973-61-6 CAPLUS
CN Cobalt(1+), dichloro(1,4,8,11-tetraazacyclotetradecane-κN1,κN4,κN8,κN11)-, (OC-6-12)- (9CI) (CA INDEX NAME)

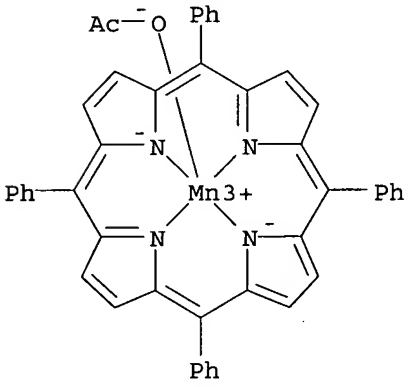


RN 89556-84-3 CAPLUS
CN Cobalt(1+), chloro(pyridine)(1,4,8,11-tetraazacyclotetradecane-N1,N4,N8,N11)-, chloride, (OC-6-23)- (9CI) (CA INDEX NAME)

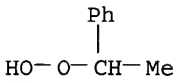


● Cl⁻

IT **58356-65-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidation **catalyst**, for aromatic olefins, benzylic alcs. by)
RN 58356-65-3 CAPLUS
CN Manganese, (acetato-κO)[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



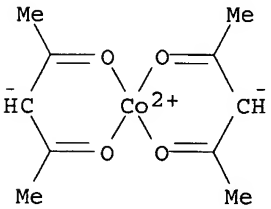
IT **3071-32-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and decomposition of)
RN 3071-32-7 CAPLUS
CN Hydroperoxide, 1-phenylethyl (9CI) (CA INDEX NAME)



L34 ANSWER 75 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:166430 CAPLUS
DOCUMENT NUMBER: 102:166430
TITLE: The liquid-phase oxidation of hydrocarbons with molecular oxygen. A selective oxidation of active cyclic methylene group to ketone group with the catalyst system composed of N,N-dialkylamides and chromium salts
AUTHOR(S): Mizukami, Fujio; Imamura, Juichi
CORPORATE SOURCE: Natl. Chem. Lab. Ind., Tsukuba, Japan
SOURCE: Kagaku Gijutsu Kenkyusho Hokoku (1984), 79(10), 515-24
CODEN: KGKHEP; ISSN: 0388-3213
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

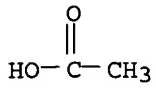
AB The metal-ion catalyzed oxidation of tetralin was carried out in solvents in which metal salts are soluble For the production of α-tetralone, a chromium salt is the best catalyst among the first-transition-metal salts and N,N-dialkylamides are the best solvents or additives. E.g., in tris(acetylacetonato)chomium(III)-catalyzed oxidation of tetralin in the presence of AcNMe2, α-tetralone was obtained in 93.0% yield with 27.2% tetralin conversion. α-Indanone and fluorenone are prepared in very high yields by analogous oxidation of indane and fluorene. The decompose of α-tetralinyl hydroperoxide with different first-transition-metal catalysts was also carried out in DMF in order to elucidate the formation mechanism for α-tetralone in the oxidation of tetralin in the presence of N,N-dialkylamides. The product distribution in the oxidation mainly depends on the decomposition mechanism of α-cyclic peroxide and that N,N-dialkylamides seem to promote the reaction of the α-cyclic peroxyl radical with low valent metal ions.

IT **14024-48-7**
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalyst**, for oxidation of tetralin with oxygen)
RN 14024-48-7 CAPLUS
CN Cobalt, bis(2,4-pentanedionato-κO,κO')-, (SP-4-1)- (9CI) (CA INDEX NAME)



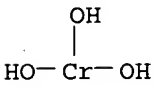
IT **1066-30-4 1308-14-1 1333-82-0**
7440-47-3D, naphthenic acid compound **7788-97-8**
10060-12-5 10101-53-8 13548-38-4
RL: **CAT (Catalyst use)**; USES (Uses)

(**catalysts**, for liquid-phase oxidation of tetralin with oxygen)
RN 1066-30-4 CAPLUS
CN Acetic acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)

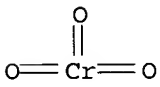


●1/3 Cr(III)

RN 1308-14-1 CAPLUS
CN Chromium hydroxide (Cr(OH)3) (8CI, 9CI) (CA INDEX NAME)



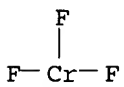
RN 1333-82-0 CAPLUS
CN Chromium oxide (CrO3) (8CI, 9CI) (CA INDEX NAME)



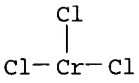
RN 7440-47-3 CAPLUS
CN Chromium (8CI, 9CI) (CA INDEX NAME)

Cr

RN 7788-97-8 CAPLUS
CN Chromium fluoride (CrF3) (6CI, 8CI, 9CI) (CA INDEX NAME)

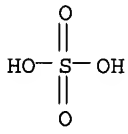


RN 10060-12-5 CAPLUS
CN Chromium chloride (CrCl3), hexahydrate (8CI, 9CI) (CA INDEX NAME)



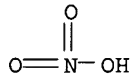
●6 H_2O

RN 10101-53-8 CAPLUS
CN Sulfuric acid, chromium(3+) salt (3:2) (6CI, 8CI, 9CI) (CA INDEX NAME)



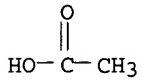
●2/3 Cr(III)

RN 13548-38-4 CAPLUS
CN Nitric acid, chromium(3+) salt (8CI, 9CI) (CA INDEX NAME)



●1/3 Cr(III)

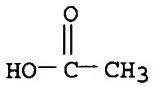
IT **638-38-0 6018-89-9 6046-93-1 6147-53-1**
7705-08-0, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts**, for oxidation of tetralin by oxygen in DMF)
RN 638-38-0 CAPLUS
CN Acetic acid, manganese(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Mn(II)

RN 6018-89-9 CAPLUS

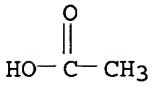
CN Acetic acid, nickel(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)



●1/2 Ni(II)

●2 H_2O

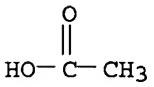
RN 6046-93-1 CAPLUS
CN Acetic acid, copper(2+) salt, monohydrate (8CI, 9CI) (CA INDEX NAME)



●1/2 Cu(II)

●1/2 H_2O

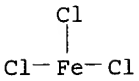
RN 6147-53-1 CAPLUS
CN Acetic acid, cobalt(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)



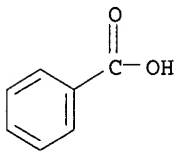
●1/2 Co(II)

●2 H_2O

RN 7705-08-0 CAPLUS
CN Iron chloride (FeCl3) (8CI, 9CI) (CA INDEX NAME)

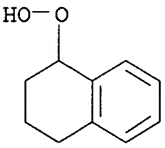


IT **932-69-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts**, for oxidation of tetralin with oxygen)
RN 932-69-4 CAPLUS
CN Benzoic acid, cobalt(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Co(II)

IT **771-29-9P**
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, from oxidation of tetralin)
RN 771-29-9 CAPLUS
CN Hydroperoxide, 1,2,3,4-tetrahydro-1-naphthalenyl (9CI) (CA INDEX NAME)



IT **7782-44-7**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(oxidation by, of tetralin)
RN 7782-44-7 CAPLUS
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

L34 ANSWER 76 OF 76 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:136128 CAPLUS
DOCUMENT NUMBER: 88:136128
TITLE: Hydrogenation of organic peroxide

INVENTOR(S): Mabuchi, Shunsuke; Tsuzuki, Kenji; Kumoi, Sadakatsu
PATENT ASSIGNEE(S): Toyo Soda Mfg. Co., Ltd., Japan
SOURCE: Ger. Offen., 22 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2731867	A1	19780119	DE 1977-2731867	19770714
DE 2731867	B2	19810702		
DE 2731867	C3	19820401		
JP 53009705	A2	19780128	JP 1976-83513	19760715
US 4123616	A	19781031	US 1977-806703	19770615
NL 7707883	A	19780117	NL 1977-7883	19770715

PRIORITY APPLN. INFO.: JP 1976-83513 A 19760715

AB Aliphatic peroxides were hydrogenated in an inert solvent using a suspended Ni catalyst at a rate of 0.05-10 g/h/g catalyst at 140-200° and H pressure 10-300 kg/cm2. Thus, butadiene peroxide polymer was hydrogenated in AcOEt at 150°, 100 kg/cm2 H to give 1,4-butanediol 53.5 and 1,2-butanediol 25.1%.

IT **7440-02-0**, uses and miscellaneous
RL: **CAT (Catalyst use)**; USES (Uses)
(**catalysts**, for hydrogenation of aliphatic peroxides to alcs.)
RN 7440-02-0 CAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

IT **30946-71-5**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrogenation of)
RN 30946-71-5 CAPLUS
CN 1,3-Butadiene, polymer with oxygen (9CI) (CA INDEX NAME)

CM 1

CRN 7782-44-7
CMF O2

O═O

CM 2

CRN 106-99-0
CMF C4 H6

H_2C═CH–CH═CH_2

IT **4676-82-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 4676-82-8 CAPLUS
CN Hydroperoxide, tetrahydro-2-furanyl (9CI) (CA INDEX NAME)